



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:50 AM UTC

PDB ID : 1AIP / pdb_00001aip
Title : EF-TU EF-TS COMPLEX FROM THERMUS THERMOPHILUS
Authors : Wang, Y.; Jiang, Y.; Meyering-Voss, M.; Sprinzl, M.; Sigler, P.B.
Deposited on : 1997-04-22
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

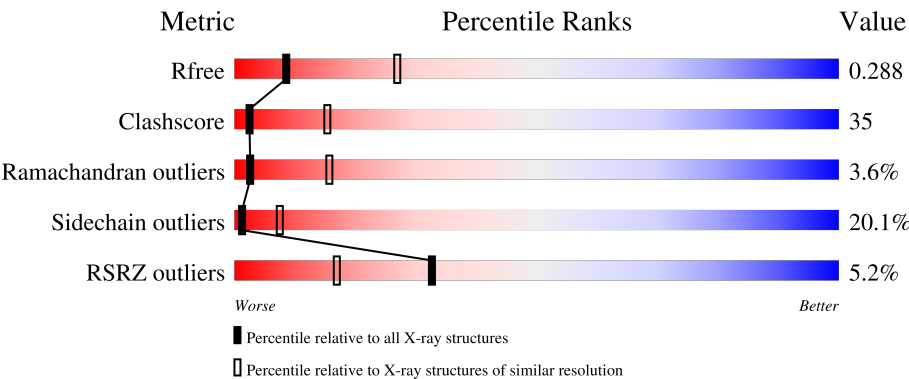
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	405	2% 44% 38% 9% 8%
1	B	405	5% 39% 39% 12% 8%
1	E	405	% 46% 36% 9% 8%
1	F	405	17% 43% 37% 11% 8%
2	C	196	38% 43% 16% ..

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Mol	Chain	Length	Quality of chain
2	D	196	3% 41% 41% 17% ..
2	G	196	0% 40% 43% 15% ..
2	H	196	5% 41% 43% 13% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17575 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ELONGATION FACTOR TU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	0	0
			2865	1810	503	541	11			
1	B	373	Total	C	N	O	S	0	0	0
			2859	1807	495	545	12			
1	E	372	Total	C	N	O	S	0	0	0
			2869	1812	502	543	12			
1	F	372	Total	C	N	O	S	0	0	0
			2841	1792	495	542	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	THR	ALA	conflict	UNP P60338
B	35	THR	ALA	conflict	UNP P60338
E	35	THR	ALA	conflict	UNP P60338
F	35	THR	ALA	conflict	UNP P60338

- Molecule 2 is a protein called ELONGATION FACTOR TS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	195	Total	C	N	O	S	0	0	0
			1544	969	276	290	9			
2	D	195	Total	C	N	O	S	0	0	0
			1513	952	268	284	9			
2	G	195	Total	C	N	O	S	0	0	0
			1546	970	279	288	9			
2	H	194	Total	C	N	O	S	0	0	0
			1523	957	274	283	9			

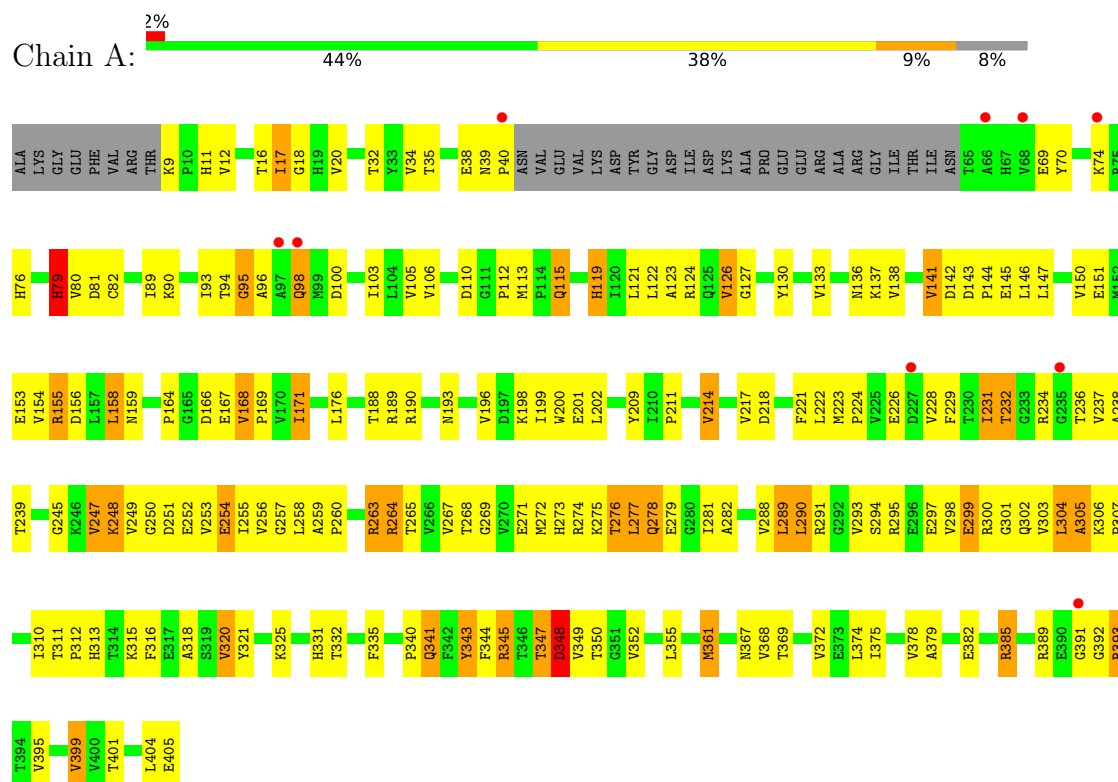
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	O 2	0	0
3	C	1	Total 1	O 1	0	0
3	D	4	Total 4	O 4	0	0
3	E	3	Total 3	O 3	0	0
3	G	4	Total 4	O 4	0	0
3	H	1	Total 1	O 1	0	0

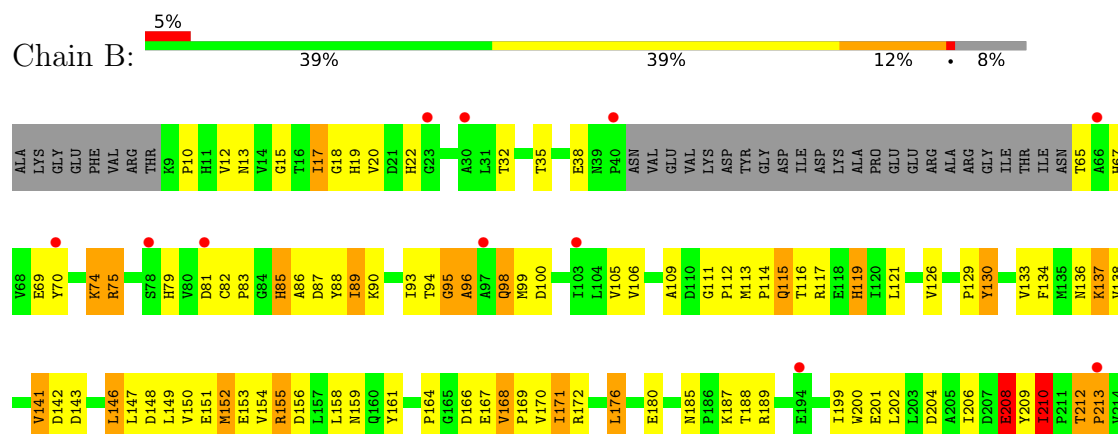
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: ELONGATION FACTOR TU

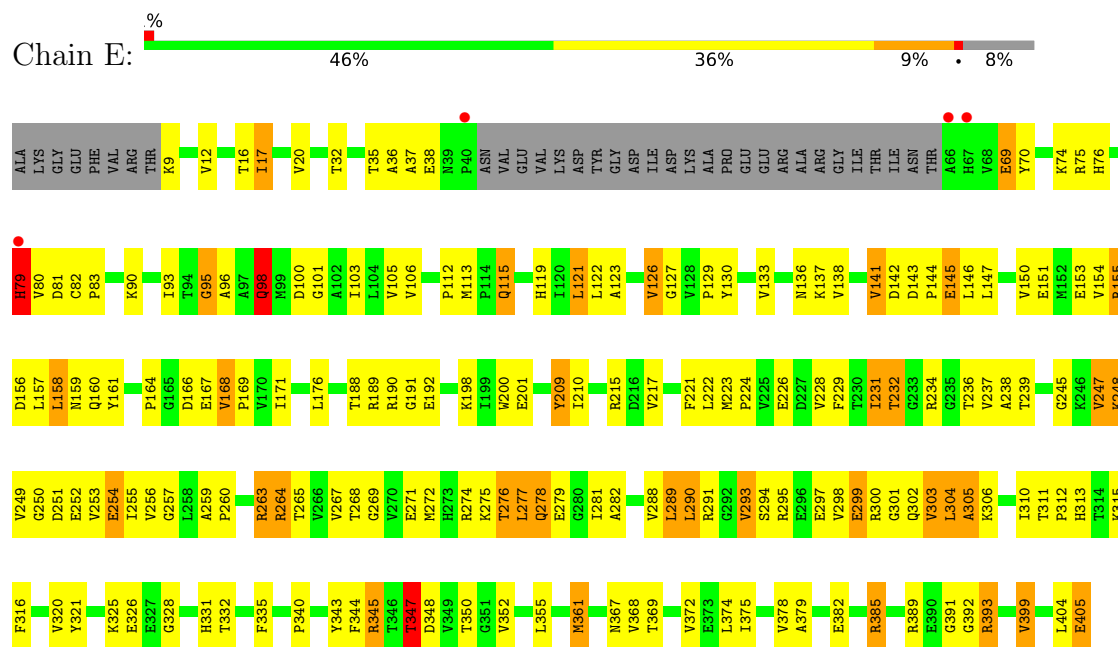


• Molecule 1: ELONGATION FACTOR TU

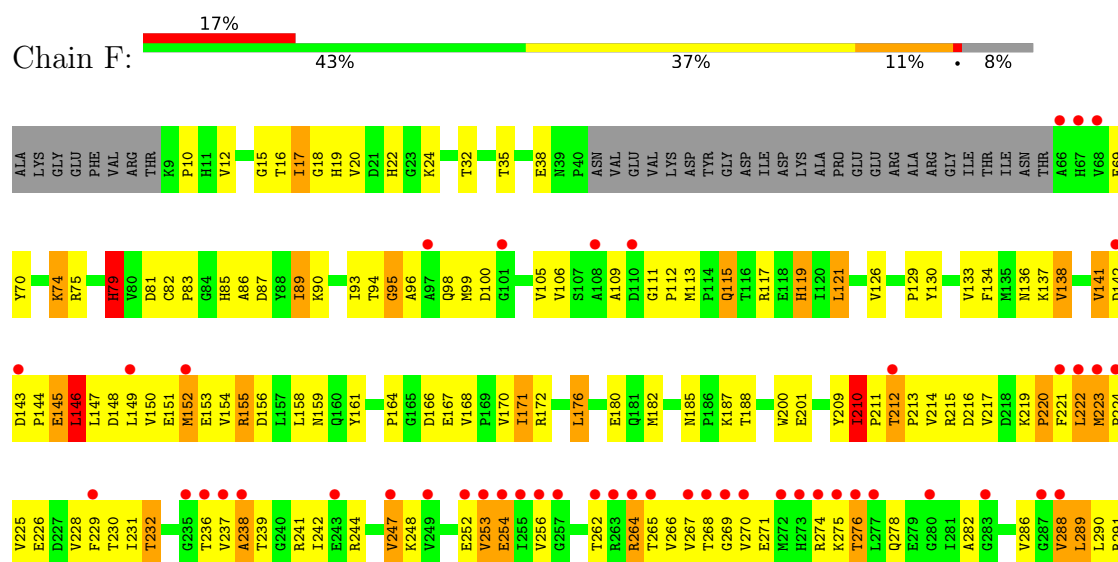


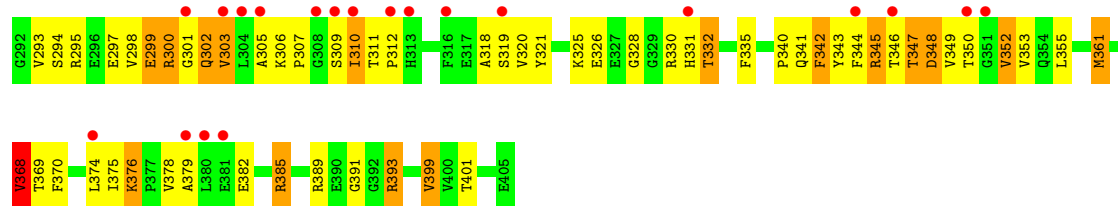


• Molecule 1: ELONGATION FACTOR TU

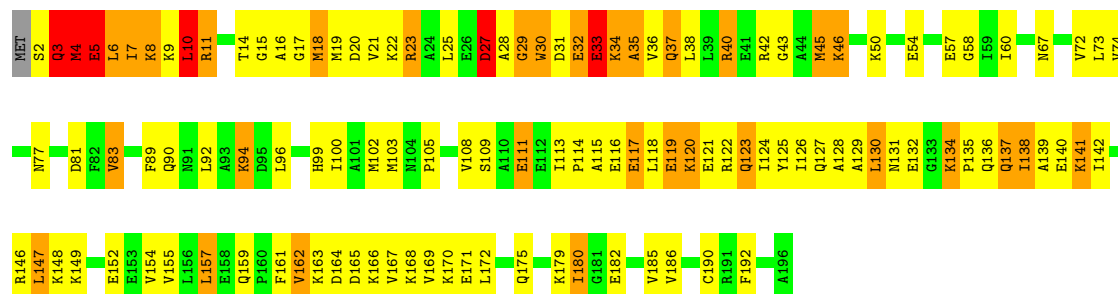


• Molecule 1: ELONGATION FACTOR TU

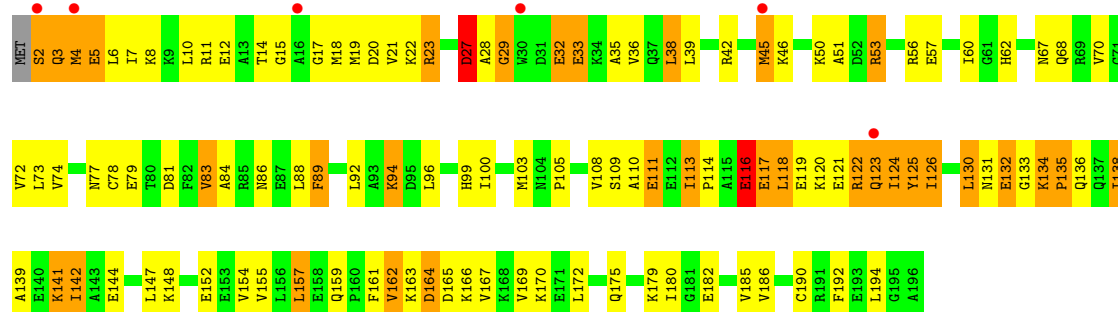




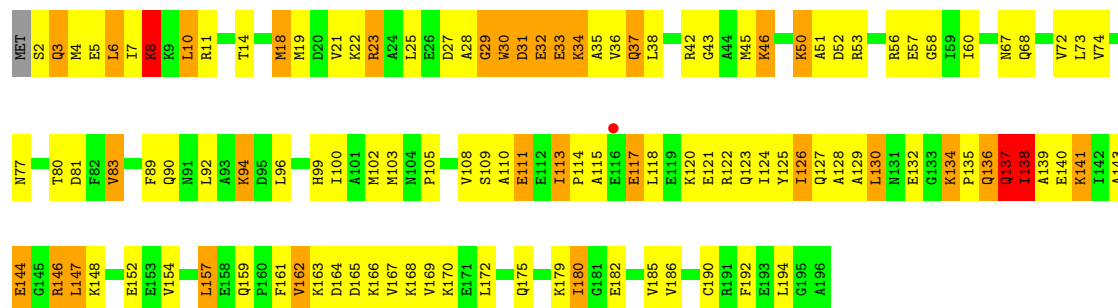
• Molecule 2: ELONGATION FACTOR TS



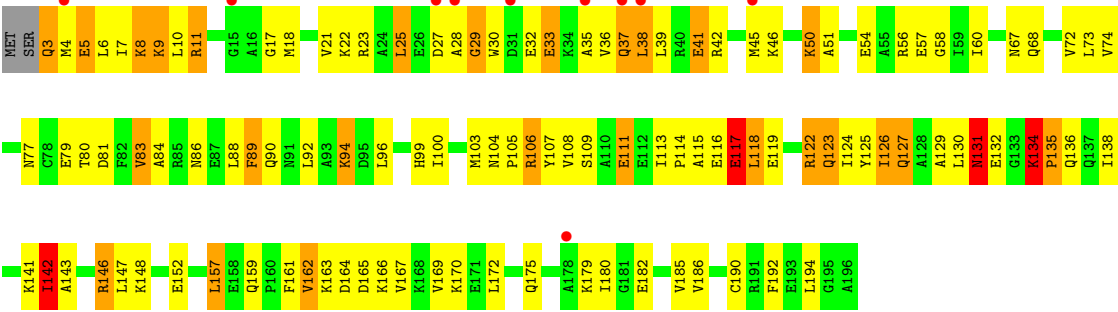
• Molecule 2: ELONGATION FACTOR TS



• Molecule 2: ELONGATION FACTOR TS



• Molecule 2: ELONGATION FACTOR TS



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	120.30Å 127.50Å 123.70Å 90.00° 90.30° 90.00°	Depositor
Resolution (Å)	100.00 – 3.00 100.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	92.0 (100.00-3.00) 92.7 (100.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 2.77Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.216 , 0.289 0.229 , 0.288	Depositor DCC
R_{free} test set	4245 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	52.9	Xtriage
Anisotropy	0.890	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 74.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for l,k,-h 0.100 for h,-k,-l 0.017 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17575	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.58	0/2922	1.05	17/3974 (0.4%)
1	B	0.51	0/2915	1.02	15/3965 (0.4%)
1	E	0.59	0/2926	1.06	20/3977 (0.5%)
1	F	0.59	0/2897	1.05	13/3941 (0.3%)
2	C	0.55	0/1562	1.00	7/2094 (0.3%)
2	D	0.51	0/1531	1.04	11/2056 (0.5%)
2	G	0.57	0/1564	0.99	4/2096 (0.2%)
2	H	0.52	0/1541	1.02	10/2067 (0.5%)
All	All	0.56	0/17858	1.03	97/24170 (0.4%)

There are no bond length outliers.

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	209	TYR	N-CA-C	8.53	122.98	112.23
2	H	113	ILE	N-CA-C	8.24	117.00	107.77
2	D	113	ILE	N-CA-C	8.09	115.94	107.76
1	F	288	VAL	N-CA-C	7.16	119.04	108.45
2	D	6	LEU	N-CA-C	-6.99	102.87	111.40
2	H	124	ILE	N-CA-C	-6.87	103.66	113.07
2	D	113	ILE	CA-C-N	6.84	126.81	120.03
2	D	113	ILE	C-N-CA	6.84	126.81	120.03
2	C	89	PHE	N-CA-C	-6.75	103.84	111.07
1	B	288	VAL	N-CA-C	6.63	117.86	108.17
1	F	79	HIS	N-CA-C	6.60	119.48	108.73
1	E	133	VAL	N-CA-C	6.33	117.59	108.48
1	F	210	ILE	N-CA-C	6.24	114.06	107.76
2	D	142	ILE	N-CA-C	-6.23	104.67	110.53
1	F	253	VAL	N-CA-C	6.21	116.39	108.82
1	F	237	VAL	N-CA-C	6.19	116.78	108.11
1	F	74	LYS	N-CA-C	6.17	117.88	111.03
1	A	79	HIS	N-CA-C	6.13	119.23	109.24
1	E	367	ASN	N-CA-C	-6.11	98.94	108.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	367	ASN	N-CA-C	-6.04	98.56	108.41
1	B	105	VAL	N-CA-C	6.03	116.04	106.88
1	A	257	GLY	N-CA-C	5.99	119.57	111.72
2	G	113	ILE	CA-C-N	5.99	127.33	119.84
2	G	113	ILE	C-N-CA	5.99	127.33	119.84
1	E	209	TYR	CA-C-N	-5.98	118.28	122.59
1	E	209	TYR	C-N-CA	-5.98	118.28	122.59
1	E	257	GLY	N-CA-C	5.94	119.50	111.72
1	B	74	LYS	N-CA-C	5.92	117.60	111.03
1	E	74	LYS	N-CA-C	5.90	117.58	111.03
2	D	38	LEU	N-CA-C	-5.88	104.23	111.40
2	G	89	PHE	N-CA-C	-5.87	104.78	111.07
2	H	117	GLU	N-CA-C	-5.87	104.29	112.45
1	F	119	HIS	N-CA-C	-5.87	104.57	110.97
1	E	168	VAL	CA-C-N	5.85	126.31	119.99
1	E	168	VAL	C-N-CA	5.85	126.31	119.99
1	E	79	HIS	N-CA-C	5.85	118.77	109.24
1	B	368	VAL	N-CA-C	5.82	115.64	108.53
2	D	124	ILE	N-CA-C	-5.82	103.90	112.04
1	B	210	ILE	CA-C-N	-5.80	114.00	119.85
1	B	210	ILE	C-N-CA	-5.80	114.00	119.85
1	E	256	VAL	N-CA-C	5.77	117.31	108.71
2	D	89	PHE	N-CA-C	-5.77	104.90	111.07
1	A	145	GLU	N-CA-C	-5.74	105.78	112.89
1	F	105	VAL	N-CA-C	5.69	115.53	106.88
1	E	9	LYS	CA-C-N	5.68	126.94	119.84
1	E	9	LYS	C-N-CA	5.68	126.94	119.84
1	F	146	LEU	N-CA-C	-5.63	104.83	110.97
2	H	38	LEU	N-CA-C	-5.62	105.07	111.14
1	B	79	HIS	N-CA-C	5.62	117.88	108.73
1	A	105	VAL	N-CA-C	5.59	115.64	107.37
2	H	129	ALA	N-CA-C	-5.58	104.48	112.13
1	E	278	GLN	N-CA-C	-5.57	104.90	110.97
1	E	347	THR	N-CA-C	5.56	118.03	110.35
2	C	115	ALA	N-CA-C	5.54	118.83	111.75
2	D	155	VAL	N-CA-C	5.51	115.73	107.51
2	H	104	ASN	CB-CA-C	-5.51	107.29	111.20
1	B	320	VAL	N-CA-C	5.50	115.53	108.82
2	H	89	PHE	N-CA-C	-5.50	105.19	111.07
2	G	117	GLU	N-CA-C	-5.49	106.09	112.89
2	H	142	ILE	N-CA-C	-5.49	104.99	113.16
2	C	130	LEU	N-CA-C	-5.44	105.43	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	LYS	N-CA-C	5.39	117.01	111.03
1	A	168	VAL	CA-C-N	5.39	125.81	119.99
1	A	168	VAL	C-N-CA	5.39	125.81	119.99
1	A	133	VAL	N-CA-C	5.38	116.23	108.48
1	A	256	VAL	N-CA-C	5.38	116.73	108.71
1	F	145	GLU	N-CA-C	-5.38	105.85	112.90
1	E	105	VAL	N-CA-C	5.37	115.31	107.37
1	B	119	HIS	N-CA-C	-5.36	105.13	110.97
1	E	145	GLU	N-CA-C	-5.33	105.51	112.23
1	B	85	HIS	N-CA-C	-5.32	105.39	111.14
1	F	368	VAL	N-CA-C	5.32	115.02	108.53
1	A	34	VAL	N-CA-C	5.32	116.09	110.72
1	A	320	VAL	N-CA-C	5.31	116.50	108.96
1	E	119	HIS	N-CA-C	-5.29	105.21	110.97
1	B	309	SER	N-CA-C	5.27	117.43	111.11
1	B	168	VAL	CA-C-N	5.27	125.68	119.99
1	B	168	VAL	C-N-CA	5.27	125.68	119.99
1	B	331	HIS	N-CA-C	-5.24	107.02	113.41
2	H	11	ARG	N-CA-C	-5.24	106.74	113.23
1	E	75	ARG	N-CA-C	5.23	116.61	109.18
1	A	9	LYS	CA-C-N	5.23	126.38	119.84
1	A	9	LYS	C-N-CA	5.23	126.38	119.84
1	B	75	ARG	N-CA-C	5.23	116.61	109.18
1	F	238	ALA	N-CA-C	5.22	116.92	108.41
1	A	119	HIS	N-CA-C	-5.18	105.32	110.97
2	C	123	GLN	N-CA-C	-5.18	106.06	112.38
2	H	50	LYS	N-CA-C	-5.16	106.98	113.28
2	C	155	VAL	N-CA-C	5.15	115.51	107.99
2	D	53	ARG	N-CA-C	-5.13	103.63	110.55
2	D	136	GLN	N-CA-C	5.12	116.55	110.97
2	C	3	GLN	N-CA-C	-5.10	105.61	111.07
1	A	305	ALA	N-CA-C	5.09	116.04	108.60
1	F	352	VAL	N-CA-C	5.07	115.21	108.11
1	E	305	ALA	N-CA-C	5.05	115.98	108.60
1	A	348	ASP	N-CA-C	-5.02	99.65	107.93
2	C	10	LEU	N-CA-C	-5.01	105.29	111.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2865	0	2847	176	0
1	B	2859	0	2835	237	0
1	E	2869	0	2855	165	0
1	F	2841	0	2802	184	0
2	C	1544	0	1558	140	0
2	D	1513	0	1507	133	0
2	G	1546	0	1565	126	0
2	H	1523	0	1530	111	0
3	A	2	0	0	0	0
3	C	1	0	0	0	0
3	D	4	0	0	0	0
3	E	3	0	0	0	0
3	G	4	0	0	0	0
3	H	1	0	0	0	0
All	All	17575	0	17499	1217	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 35.

All (1217) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:ARG:HH11	1:B:264:ARG:HG2	1.19	1.07
1:F:95:GLY:HA2	1:F:385:ARG:HH21	1.18	1.04
1:A:341:GLN:HB3	1:A:343:TYR:HE1	1.25	1.02
1:B:228:VAL:HG21	1:B:298:VAL:HG12	1.42	1.01
1:B:75:ARG:HH11	1:B:212:THR:HG23	1.26	1.00
1:B:95:GLY:HA2	1:B:385:ARG:HH21	1.24	0.99
1:A:95:GLY:HA2	1:A:385:ARG:HH21	1.27	0.98
1:B:232:THR:HG21	2:G:110:ALA:HB1	1.46	0.98
1:A:130:TYR:CE2	1:A:211:PRO:HD2	1.99	0.96
2:C:3:GLN:HE21	2:C:3:GLN:HA	1.30	0.95
1:F:341:GLN:NE2	1:F:391:GLY:H	1.64	0.95
1:F:298:VAL:HA	1:F:302:GLN:HE22	1.28	0.94
1:B:223:MET:HE2	1:B:304:LEU:HD21	1.49	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:MET:HE2	1:A:304:LEU:HD21	1.46	0.94
1:F:341:GLN:HE22	1:F:391:GLY:H	1.06	0.93
1:F:95:GLY:HA2	1:F:385:ARG:NH2	1.83	0.93
2:H:11:ARG:HB2	2:H:21:VAL:HG21	1.49	0.92
2:C:33:GLU:CD	2:C:33:GLU:H	1.79	0.91
1:F:228:VAL:HG21	1:F:298:VAL:HG12	1.51	0.91
1:F:95:GLY:CA	1:F:385:ARG:HE	1.84	0.90
2:C:135:PRO:HG2	2:C:138:ILE:HB	1.52	0.89
1:B:224:PRO:HA	1:B:303:VAL:HG23	1.54	0.89
1:F:264:ARG:HG2	1:F:264:ARG:HH11	1.36	0.89
2:C:34:LYS:HD3	2:C:34:LYS:N	1.86	0.89
1:A:263:ARG:HH12	1:A:297:GLU:HB3	1.37	0.88
1:B:95:GLY:HA2	1:B:385:ARG:NH2	1.88	0.88
1:F:224:PRO:HA	1:F:303:VAL:HG23	1.57	0.87
2:H:161:PHE:CE2	2:H:163:LYS:HB2	2.10	0.87
1:F:368:VAL:HG12	1:F:369:THR:H	1.38	0.86
1:A:224:PRO:HA	1:A:303:VAL:HG23	1.56	0.86
2:C:73:LEU:HG	2:D:73:LEU:HG	1.59	0.85
2:D:3:GLN:HG2	2:D:4:MET:H	1.41	0.85
1:E:255:ILE:HD12	1:E:263:ARG:HG2	1.59	0.85
1:B:306:LYS:O	1:B:309:SER:HB2	1.75	0.85
1:E:224:PRO:HA	1:E:303:VAL:HG23	1.57	0.85
2:D:130:LEU:HD13	2:D:135:PRO:HA	1.57	0.85
2:C:121:GLU:HA	2:C:124:ILE:HD12	1.57	0.84
2:D:122:ARG:HH21	2:D:126:ILE:HD11	1.41	0.84
2:D:125:TYR:HE2	2:D:147:LEU:HD23	1.41	0.84
2:C:33:GLU:O	2:C:37:GLN:HB2	1.78	0.83
2:C:6:LEU:HD22	2:C:25:LEU:HD22	1.61	0.83
1:A:341:GLN:HB3	1:A:343:TYR:CE1	2.13	0.83
2:G:146:ARG:HG3	2:G:146:ARG:HH11	1.42	0.83
2:H:3:GLN:HE22	2:H:30:TRP:HE3	1.24	0.83
1:B:368:VAL:HG12	1:B:369:THR:H	1.41	0.83
1:B:86:ALA:O	1:B:89:ILE:HG22	1.79	0.83
2:H:122:ARG:O	2:H:125:TYR:HB2	1.79	0.83
1:F:141:VAL:HG21	1:F:147:LEU:HD21	1.61	0.82
2:H:21:VAL:O	2:H:25:LEU:HD12	1.78	0.82
2:H:125:TYR:HA	2:H:146:ARG:HH12	1.44	0.82
1:B:95:GLY:N	1:B:385:ARG:HE	1.76	0.82
1:E:95:GLY:HA2	1:E:385:ARG:HH21	1.43	0.82
1:F:253:VAL:HG22	1:F:254:GLU:H	1.45	0.82
2:D:161:PHE:CE2	2:D:163:LYS:HB2	2.15	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:GLY:CA	1:B:385:ARG:HE	1.92	0.81
1:B:298:VAL:HA	1:B:302:GLN:HE22	1.44	0.81
1:E:223:MET:HE2	1:E:304:LEU:HD21	1.60	0.81
1:F:95:GLY:N	1:F:385:ARG:HE	1.77	0.81
1:E:263:ARG:HG3	1:E:264:ARG:N	1.94	0.81
2:G:73:LEU:HB2	2:G:190:CYS:HB3	1.64	0.80
1:E:343:TYR:CZ	1:E:389:ARG:HD2	2.17	0.79
1:B:141:VAL:HG21	1:B:147:LEU:HD21	1.64	0.79
1:A:16:THR:HG23	1:A:79:HIS:HE1	1.47	0.79
2:C:73:LEU:HB2	2:C:190:CYS:HB3	1.65	0.79
2:C:118:LEU:HD12	2:C:119:GLU:N	1.98	0.79
2:D:73:LEU:HB2	2:D:190:CYS:HB3	1.63	0.79
1:B:290:LEU:HB2	1:B:293:VAL:HG21	1.64	0.78
2:C:161:PHE:CE2	2:C:163:LYS:HB2	2.17	0.78
1:B:263:ARG:HH11	1:B:263:ARG:HB3	1.49	0.78
1:F:320:VAL:HG12	1:F:321:TYR:N	1.99	0.78
2:C:137:GLN:H	2:C:137:GLN:HE21	1.29	0.78
2:G:73:LEU:HG	2:H:73:LEU:HG	1.65	0.78
1:A:226:GLU:O	1:A:300:ARG:HB2	1.83	0.77
1:B:264:ARG:HG2	1:B:264:ARG:NH1	1.94	0.77
2:C:7:ILE:HG22	2:C:21:VAL:HG12	1.66	0.77
2:H:108:VAL:O	2:H:157:LEU:HD22	1.85	0.77
1:B:295:ARG:HG3	1:B:295:ARG:HH11	1.48	0.77
2:G:161:PHE:CE2	2:G:163:LYS:HB2	2.20	0.76
2:D:118:LEU:O	2:D:118:LEU:HD12	1.85	0.76
2:H:7:ILE:HD11	2:H:22:LYS:HG3	1.65	0.76
2:H:7:ILE:O	2:H:11:ARG:HB3	1.86	0.76
2:H:130:LEU:HA	2:H:134:LYS:O	1.84	0.76
1:A:368:VAL:HG12	1:A:369:THR:H	1.49	0.76
2:C:7:ILE:HG22	2:C:21:VAL:CG1	2.16	0.76
2:D:10:LEU:HD21	2:D:36:VAL:HG12	1.66	0.76
1:E:368:VAL:HG12	1:E:369:THR:H	1.50	0.76
1:B:226:GLU:O	1:B:300:ARG:HB2	1.86	0.75
1:E:226:GLU:O	1:E:300:ARG:HB2	1.86	0.75
1:F:268:THR:OG1	1:F:291:ARG:HG3	1.86	0.75
2:G:10:LEU:CD1	2:G:25:LEU:HD21	2.17	0.75
2:C:129:ALA:O	2:C:134:LYS:HB2	1.87	0.75
1:F:75:ARG:HH11	1:F:212:THR:HG23	1.52	0.75
1:B:290:LEU:N	1:B:290:LEU:HD22	2.02	0.75
2:H:125:TYR:HB3	2:H:143:ALA:HB1	1.68	0.75
1:B:289:LEU:C	1:B:290:LEU:HD13	2.12	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:10:LEU:HD12	2:D:21:VAL:HG13	1.69	0.74
1:B:320:VAL:HG12	1:B:321:TYR:H	1.52	0.74
1:F:320:VAL:HG12	1:F:321:TYR:H	1.51	0.74
1:B:115:GLN:HG2	2:D:83:VAL:CG2	2.17	0.74
1:F:115:GLN:HG2	2:H:83:VAL:CG2	2.17	0.74
2:G:3:GLN:HE21	2:G:3:GLN:HA	1.53	0.74
2:H:125:TYR:CE2	2:H:146:ARG:HD2	2.23	0.74
2:D:32:GLU:CD	2:D:32:GLU:H	1.94	0.73
1:A:16:THR:HG23	1:A:79:HIS:CE1	2.23	0.73
1:F:264:ARG:HG2	1:F:264:ARG:NH1	2.03	0.73
1:B:320:VAL:HG12	1:B:321:TYR:N	2.04	0.73
1:A:115:GLN:H	1:A:115:GLN:HE21	1.36	0.73
1:F:130:TYR:CE2	1:F:209:TYR:HB3	2.23	0.73
1:E:222:LEU:C	1:E:222:LEU:HD23	2.14	0.73
1:E:16:THR:HG23	1:E:79:HIS:CE1	2.24	0.73
2:H:73:LEU:HB2	2:H:190:CYS:HB3	1.69	0.73
1:A:115:GLN:H	1:A:115:GLN:NE2	1.87	0.72
1:A:130:TYR:HB3	1:A:209:TYR:CE2	2.24	0.72
1:E:115:GLN:H	1:E:115:GLN:HE21	1.36	0.72
1:F:228:VAL:HG22	1:F:238:ALA:HB2	1.71	0.72
1:A:237:VAL:HG22	1:A:289:LEU:HB3	1.70	0.72
2:D:108:VAL:O	2:D:157:LEU:HD22	1.90	0.72
1:B:115:GLN:H	1:B:115:GLN:HE21	1.37	0.72
1:B:156:ASP:HA	1:B:159:ASN:HD22	1.53	0.72
1:E:320:VAL:HG12	1:E:321:TYR:N	2.05	0.72
1:F:113:MET:HB3	1:F:115:GLN:HE22	1.54	0.72
1:A:344:PHE:O	1:A:345:ARG:HB2	1.90	0.72
1:B:385:ARG:HH11	1:B:385:ARG:HB2	1.55	0.72
1:A:164:PRO:HB2	1:A:167:GLU:HB2	1.72	0.72
1:F:156:ASP:HA	1:F:159:ASN:HD22	1.53	0.71
1:A:343:TYR:CZ	1:A:389:ARG:HD2	2.25	0.71
1:F:224:PRO:HD2	1:F:241:ARG:O	1.90	0.71
1:E:16:THR:HG23	1:E:79:HIS:HE1	1.54	0.71
1:B:115:GLN:HG2	2:D:83:VAL:HG22	1.72	0.71
1:B:341:GLN:O	1:B:388:ILE:HA	1.91	0.71
1:B:164:PRO:HB2	1:B:167:GLU:HB2	1.73	0.71
1:B:268:THR:OG1	1:B:291:ARG:HG3	1.91	0.71
1:E:115:GLN:H	1:E:115:GLN:NE2	1.89	0.71
1:F:368:VAL:HG12	1:F:369:THR:N	2.06	0.71
2:C:137:GLN:H	2:C:137:GLN:NE2	1.88	0.70
1:E:237:VAL:HG22	1:E:289:LEU:HB3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:7:ILE:HG23	2:H:21:VAL:HB	1.72	0.70
1:A:231:ILE:HG22	1:A:231:ILE:O	1.91	0.70
1:F:385:ARG:HH11	1:F:385:ARG:HB2	1.56	0.70
2:G:2:SER:O	2:G:6:LEU:HB2	1.91	0.70
2:G:28:ALA:O	2:G:29:GLY:O	2.08	0.70
1:F:115:GLN:H	1:F:115:GLN:HE21	1.38	0.70
1:E:385:ARG:HG3	1:E:399:VAL:HG12	1.73	0.70
1:E:231:ILE:HG22	1:E:231:ILE:O	1.89	0.70
1:F:236:THR:HG21	1:F:294:SER:C	2.16	0.70
2:C:28:ALA:O	2:C:29:GLY:O	2.10	0.70
1:B:236:THR:HG21	1:B:294:SER:C	2.16	0.70
1:F:342:PHE:N	1:F:342:PHE:CD1	2.57	0.70
2:D:4:MET:O	2:D:8:LYS:HB2	1.92	0.69
2:G:123:GLN:HA	2:G:126:ILE:HG12	1.74	0.69
1:B:206:ILE:O	1:B:210:ILE:HB	1.91	0.69
2:D:96:LEU:O	2:D:100:ILE:HG13	1.92	0.69
1:A:268:THR:OG1	1:A:291:ARG:HG3	1.93	0.69
2:D:122:ARG:O	2:D:125:TYR:HB2	1.93	0.69
1:E:268:THR:OG1	1:E:291:ARG:HG3	1.92	0.69
1:B:368:VAL:HG12	1:B:369:THR:N	2.08	0.69
2:C:149:LYS:HD2	1:E:192:GLU:O	1.93	0.69
1:F:344:PHE:O	1:F:345:ARG:HB2	1.91	0.69
1:A:344:PHE:O	1:A:347:THR:HG23	1.92	0.69
1:B:344:PHE:O	1:B:345:ARG:HB2	1.91	0.69
2:C:34:LYS:HD3	2:C:34:LYS:H	1.57	0.69
1:E:344:PHE:O	1:E:347:THR:HG23	1.93	0.69
1:B:254:GLU:OE1	1:B:307:PRO:HA	1.93	0.69
1:B:301:GLY:HA2	1:B:347:THR:HG22	1.75	0.68
2:C:32:GLU:O	2:C:35:ALA:N	2.26	0.68
1:A:113:MET:HB3	1:A:115:GLN:HE22	1.58	0.68
1:F:143:ASP:OD1	1:F:145:GLU:HB2	1.93	0.68
1:F:115:GLN:HG2	2:H:83:VAL:HG22	1.75	0.68
1:A:313:HIS:HB3	1:A:405:GLU:OXT	1.94	0.68
1:B:115:GLN:H	1:B:115:GLN:NE2	1.91	0.68
1:A:222:LEU:HD23	1:A:222:LEU:C	2.19	0.68
2:C:2:SER:HB3	2:C:5:GLU:HB2	1.76	0.68
1:F:254:GLU:OE1	1:F:307:PRO:HA	1.94	0.68
2:G:108:VAL:O	2:G:157:LEU:HD22	1.94	0.68
1:B:236:THR:OG1	1:B:293:VAL:HG23	1.94	0.67
2:C:108:VAL:O	2:C:157:LEU:HD22	1.94	0.67
2:H:138:ILE:HG22	2:H:142:ILE:HD12	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3:GLN:CG	2:D:4:MET:H	2.06	0.67
1:E:146:LEU:O	1:E:150:VAL:HG23	1.94	0.67
1:A:289:LEU:C	1:A:290:LEU:HD13	2.20	0.67
1:A:298:VAL:HA	1:A:302:GLN:HE22	1.59	0.67
2:G:123:GLN:HA	2:G:126:ILE:CG1	2.24	0.67
1:B:216:ASP:HA	1:B:219:LYS:HD2	1.77	0.67
1:A:277:LEU:HD23	1:A:278:GLN:OE1	1.95	0.67
1:B:113:MET:HB3	1:B:115:GLN:HE22	1.59	0.67
1:B:253:VAL:HG22	1:B:254:GLU:H	1.60	0.67
2:H:96:LEU:O	2:H:100:ILE:HG13	1.95	0.67
1:E:368:VAL:HG12	1:E:369:THR:N	2.09	0.67
2:G:113:ILE:HG23	2:G:114:PRO:HD2	1.76	0.67
1:A:320:VAL:HG12	1:A:321:TYR:N	2.09	0.66
2:C:6:LEU:HD13	2:C:30:TRP:CE3	2.30	0.66
2:D:131:ASN:O	2:D:133:GLY:N	2.26	0.66
2:G:11:ARG:HB2	2:G:21:VAL:HG21	1.77	0.66
1:A:291:ARG:HB2	1:A:291:ARG:HH11	1.60	0.66
2:C:99:HIS:HD2	2:C:162:VAL:H	1.44	0.66
2:D:134:LYS:HD2	2:D:134:LYS:N	2.11	0.66
1:F:113:MET:HB3	1:F:115:GLN:NE2	2.09	0.66
2:D:23:ARG:O	2:D:27:ASP:HB2	1.94	0.66
2:D:134:LYS:HB2	2:D:138:ILE:HB	1.78	0.66
1:A:385:ARG:HG3	1:A:399:VAL:HG12	1.77	0.66
2:D:99:HIS:HD2	2:D:162:VAL:H	1.43	0.66
1:F:318:ALA:HA	1:F:401:THR:HG23	1.78	0.66
1:E:344:PHE:O	1:E:345:ARG:HB2	1.96	0.66
2:C:6:LEU:HD13	2:C:30:TRP:HE3	1.61	0.66
1:F:115:GLN:H	1:F:115:GLN:NE2	1.94	0.65
2:G:96:LEU:O	2:G:100:ILE:HG13	1.96	0.65
1:E:113:MET:HB3	1:E:115:GLN:HE22	1.61	0.65
1:A:263:ARG:HH22	1:A:297:GLU:HG2	1.61	0.65
2:D:3:GLN:OE1	2:D:5:GLU:HB2	1.96	0.65
1:A:368:VAL:HG12	1:A:369:THR:N	2.11	0.65
1:B:113:MET:HB3	1:B:115:GLN:NE2	2.11	0.65
1:E:247:VAL:HG13	1:E:247:VAL:O	1.95	0.65
1:E:17:ILE:HD13	1:E:17:ILE:H	1.62	0.65
2:G:10:LEU:HD13	2:G:25:LEU:HD11	1.78	0.65
2:H:42:ARG:HA	2:H:45:MET:HE3	1.79	0.65
1:A:95:GLY:HA2	1:A:385:ARG:NH2	2.06	0.64
1:E:290:LEU:HD22	1:E:290:LEU:N	2.11	0.64
1:E:298:VAL:HA	1:E:302:GLN:HE22	1.60	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:253:VAL:HG22	1:F:254:GLU:N	2.12	0.64
1:A:90:LYS:O	1:A:94:THR:HG23	1.98	0.64
1:B:267:VAL:HG12	1:B:269:GLY:H	1.62	0.64
1:A:290:LEU:N	1:A:290:LEU:HD22	2.12	0.64
1:B:141:VAL:HG21	1:B:147:LEU:CD2	2.27	0.64
1:F:141:VAL:HG21	1:F:147:LEU:CD2	2.27	0.64
1:F:228:VAL:HG22	1:F:238:ALA:CB	2.27	0.64
1:A:224:PRO:CA	1:A:303:VAL:HG23	2.28	0.64
1:B:318:ALA:HA	1:B:401:THR:HG23	1.80	0.64
2:D:3:GLN:HG2	2:D:4:MET:N	2.12	0.64
2:D:134:LYS:HG3	2:D:142:ILE:HD11	1.79	0.64
2:C:28:ALA:HB2	2:C:38:LEU:HD22	1.79	0.64
2:D:130:LEU:O	2:D:130:LEU:HD12	1.98	0.64
1:F:210:ILE:HG13	1:F:210:ILE:O	1.98	0.64
1:F:220:PRO:O	1:F:244:ARG:HG3	1.98	0.64
1:F:236:THR:OG1	1:F:293:VAL:HG23	1.98	0.64
1:A:93:ILE:C	1:A:95:GLY:H	2.07	0.63
2:C:3:GLN:HA	2:C:3:GLN:NE2	2.10	0.63
1:F:141:VAL:CG2	1:F:147:LEU:HD21	2.29	0.63
2:G:42:ARG:HA	2:G:45:MET:HE3	1.79	0.63
1:A:304:LEU:CD2	1:A:304:LEU:H	2.12	0.63
2:C:129:ALA:HB3	2:C:139:ALA:HB1	1.80	0.63
1:E:93:ILE:C	1:E:95:GLY:H	2.07	0.63
2:C:142:ILE:HG23	1:E:191:GLY:HA2	1.81	0.63
1:F:130:TYR:HE2	1:F:209:TYR:HB3	1.64	0.63
1:F:236:THR:HG21	1:F:295:ARG:N	2.13	0.63
1:A:16:THR:CG2	1:A:79:HIS:HE1	2.12	0.63
1:E:291:ARG:HB2	1:E:291:ARG:HH11	1.62	0.62
2:H:99:HIS:HD2	2:H:162:VAL:H	1.46	0.62
1:B:232:THR:HG21	2:G:110:ALA:CB	2.23	0.62
2:G:146:ARG:HG3	2:G:146:ARG:NH1	2.07	0.62
1:B:100:ASP:O	1:B:129:PRO:HG2	2.00	0.62
2:C:31:ASP:OD2	2:C:34:LYS:HE3	1.99	0.62
2:D:122:ARG:NH2	2:D:126:ILE:HD11	2.12	0.62
1:E:289:LEU:C	1:E:290:LEU:HD13	2.24	0.62
1:B:263:ARG:NH2	1:B:297:GLU:HB3	2.14	0.62
1:E:16:THR:CG2	1:E:79:HIS:HE1	2.12	0.62
1:A:263:ARG:HG3	1:A:264:ARG:N	2.13	0.62
2:H:5:GLU:HG3	2:H:9:LYS:HE2	1.82	0.62
1:A:236:THR:HG21	1:A:295:ARG:N	2.15	0.62
1:B:141:VAL:CG2	1:B:147:LEU:HD21	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:34:LYS:HZ3	2:C:34:LYS:HB2	1.65	0.62
1:E:304:LEU:CD2	1:E:304:LEU:H	2.12	0.62
1:F:95:GLY:CA	1:F:385:ARG:NE	2.61	0.62
1:B:220:PRO:O	1:B:244:ARG:HG3	2.00	0.62
1:B:221:PHE:O	1:B:305:ALA:HB1	2.00	0.62
2:H:114:PRO:HG2	2:H:117:GLU:HB2	1.82	0.61
2:C:119:GLU:OE1	2:C:119:GLU:HA	1.99	0.61
2:D:3:GLN:CG	2:D:4:MET:N	2.64	0.61
2:D:139:ALA:HA	2:D:142:ILE:HB	1.82	0.61
1:B:304:LEU:H	1:B:304:LEU:CD2	2.12	0.61
2:G:113:ILE:CG2	2:G:114:PRO:HD2	2.29	0.61
2:G:141:LYS:O	2:G:144:GLU:HB2	2.01	0.61
2:D:121:GLU:HA	2:D:124:ILE:HD12	1.83	0.61
1:F:171:ILE:HD12	1:F:171:ILE:N	2.16	0.61
1:A:171:ILE:HD12	1:A:171:ILE:N	2.16	0.61
2:C:43:GLY:HA2	2:C:46:LYS:HG3	1.82	0.61
1:E:115:GLN:HG2	2:G:83:VAL:CG2	2.30	0.61
1:A:17:ILE:HD13	1:A:17:ILE:H	1.66	0.61
1:F:291:ARG:NH1	1:F:291:ARG:HB2	2.16	0.61
1:B:75:ARG:HH22	1:B:210:ILE:CG2	2.14	0.61
2:D:134:LYS:HB2	2:D:138:ILE:HD12	1.82	0.61
2:H:8:LYS:HG3	2:H:9:LYS:HG2	1.83	0.61
2:H:7:ILE:CD1	2:H:22:LYS:HG3	2.30	0.60
1:B:204:ASP:O	1:B:208:GLU:HG2	2.00	0.60
2:G:125:TYR:HE2	2:G:147:LEU:HD23	1.66	0.60
1:B:171:ILE:N	1:B:171:ILE:HD12	2.16	0.60
2:C:90:GLN:HE22	2:D:68:GLN:HE22	1.47	0.60
1:A:113:MET:HB3	1:A:115:GLN:NE2	2.16	0.60
1:A:263:ARG:NH1	1:A:297:GLU:HB3	2.12	0.60
2:C:31:ASP:HB3	2:C:34:LYS:NZ	2.16	0.60
1:F:164:PRO:HB2	1:F:167:GLU:HB2	1.82	0.60
2:H:33:GLU:C	2:H:35:ALA:H	2.08	0.60
1:A:295:ARG:HG3	1:A:295:ARG:HH11	1.66	0.60
1:F:95:GLY:HA2	1:F:385:ARG:CZ	2.31	0.60
2:G:10:LEU:HD12	2:G:25:LEU:HD21	1.82	0.60
1:A:255:ILE:HD12	1:A:263:ARG:HG2	1.82	0.60
2:G:114:PRO:HG2	2:G:117:GLU:HB3	1.84	0.60
2:G:136:GLN:O	2:G:138:ILE:N	2.34	0.60
1:B:228:VAL:HG22	1:B:238:ALA:HB2	1.83	0.60
2:C:96:LEU:O	2:C:100:ILE:HG13	2.02	0.60
2:C:3:GLN:O	2:C:6:LEU:HB2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:14:THR:CG2	2:C:40:ARG:HH12	2.15	0.59
1:F:226:GLU:O	1:F:300:ARG:HB2	2.01	0.59
1:B:342:PHE:CD1	1:B:342:PHE:N	2.68	0.59
2:C:111:GLU:CD	2:C:111:GLU:H	2.09	0.59
2:C:120:LYS:HZ3	2:C:121:GLU:N	2.00	0.59
1:F:100:ASP:O	1:F:129:PRO:HG2	2.02	0.59
1:A:350:THR:HB	1:A:375:ILE:HD13	1.83	0.59
2:G:57:GLU:O	2:G:77:ASN:HA	2.02	0.59
1:B:75:ARG:HH11	1:B:212:THR:CG2	2.08	0.59
2:D:19:MET:HB3	2:D:23:ARG:NH1	2.17	0.59
1:B:295:ARG:HG3	1:B:295:ARG:NH1	2.17	0.59
2:D:141:LYS:HE3	2:D:144:GLU:CB	2.33	0.59
1:F:115:GLN:HG2	2:H:83:VAL:HG23	1.83	0.59
2:D:125:TYR:HE2	2:D:147:LEU:CD2	2.14	0.59
1:F:290:LEU:CB	1:F:293:VAL:HG21	2.33	0.59
1:A:291:ARG:HB2	1:A:291:ARG:NH1	2.16	0.59
2:C:148:LYS:O	2:C:152:GLU:HG3	2.03	0.59
2:G:99:HIS:HD2	2:G:162:VAL:H	1.51	0.59
1:A:347:THR:OG1	1:A:348:ASP:N	2.32	0.59
1:B:290:LEU:HB2	1:B:293:VAL:CG2	2.32	0.59
1:E:290:LEU:HB2	1:E:293:VAL:HG21	1.84	0.59
1:B:146:LEU:CD2	2:D:18:MET:HG3	2.33	0.58
1:E:291:ARG:HB2	1:E:291:ARG:NH1	2.18	0.58
1:A:385:ARG:HH11	1:A:385:ARG:HB2	1.68	0.58
1:E:325:LYS:HD2	1:E:331:HIS:ND1	2.18	0.58
1:E:236:THR:HG21	1:E:295:ARG:N	2.19	0.58
1:F:109:ALA:O	2:H:18:MET:HB3	2.03	0.58
2:G:34:LYS:HE3	2:G:34:LYS:N	2.19	0.58
1:B:18:GLY:HA2	1:B:119:HIS:CD2	2.38	0.58
1:B:231:ILE:O	1:B:231:ILE:HG22	2.02	0.58
2:D:125:TYR:CE2	2:D:147:LEU:HD23	2.30	0.58
1:E:335:PHE:CE2	1:E:361:MET:HB2	2.39	0.58
1:F:212:THR:HG22	1:F:213:PRO:HD2	1.84	0.58
1:B:154:VAL:O	1:B:158:LEU:HD12	2.04	0.58
1:E:224:PRO:CA	1:E:303:VAL:HG23	2.30	0.58
1:F:18:GLY:HA2	1:F:119:HIS:CD2	2.38	0.58
1:A:325:LYS:HD2	1:A:331:HIS:ND1	2.18	0.58
1:B:347:THR:OG1	1:B:348:ASP:N	2.34	0.58
2:C:31:ASP:O	2:C:34:LYS:NZ	2.36	0.58
2:D:2:SER:HB2	2:D:3:GLN:NE2	2.18	0.58
1:F:343:TYR:CE1	1:F:345:ARG:O	2.57	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:192:PHE:HB3	2:H:60:ILE:HD12	1.86	0.58
2:H:7:ILE:HG12	2:H:25:LEU:CD1	2.34	0.58
1:E:320:VAL:HG12	1:E:321:TYR:H	1.65	0.58
1:F:326:GLU:C	1:F:328:GLY:H	2.10	0.57
2:C:19:MET:HB3	2:C:23:ARG:NH1	2.19	0.57
1:B:293:VAL:HA	1:B:297:GLU:OE1	2.03	0.57
1:F:320:VAL:CG1	1:F:321:TYR:N	2.67	0.57
1:A:221:PHE:O	1:A:305:ALA:HB1	2.04	0.57
1:F:16:THR:HG23	1:F:79:HIS:CE1	2.39	0.57
1:F:310:ILE:HD13	1:F:379:ALA:HB1	1.86	0.57
1:A:35:THR:HG21	1:A:70:TYR:HB2	1.85	0.57
2:G:135:PRO:HG2	2:G:137:GLN:OE1	2.05	0.57
2:H:125:TYR:CZ	2:H:147:LEU:HD23	2.39	0.57
2:D:3:GLN:O	2:D:7:ILE:HG13	2.04	0.57
1:E:222:LEU:HD23	1:E:223:MET:N	2.20	0.57
1:A:293:VAL:HA	1:A:297:GLU:OE1	2.04	0.57
1:E:143:ASP:OD1	1:E:145:GLU:HB2	2.04	0.57
1:E:171:ILE:N	1:E:171:ILE:HD12	2.20	0.57
1:F:221:PHE:O	1:F:305:ALA:HB1	2.05	0.57
1:F:325:LYS:HD2	1:F:331:HIS:ND1	2.19	0.57
1:B:115:GLN:HG2	2:D:83:VAL:HG23	1.87	0.57
1:B:310:ILE:HD13	1:B:379:ALA:HB1	1.87	0.57
2:C:141:LYS:HD2	2:C:141:LYS:N	2.20	0.57
1:F:95:GLY:HA2	1:F:385:ARG:HE	1.67	0.57
2:D:99:HIS:HE1	2:D:159:GLN:OE1	1.87	0.57
2:D:138:ILE:O	2:D:142:ILE:HG13	2.04	0.57
1:E:113:MET:HB3	1:E:115:GLN:NE2	2.19	0.57
1:E:122:LEU:O	1:E:126:VAL:HG13	2.05	0.57
2:G:3:GLN:HE21	2:G:3:GLN:CA	2.15	0.57
2:H:99:HIS:HE1	2:H:159:GLN:OE1	1.88	0.57
1:B:253:VAL:HG22	1:B:254:GLU:N	2.19	0.57
2:D:111:GLU:H	2:D:111:GLU:CD	2.12	0.57
1:E:385:ARG:CG	1:E:385:ARG:HH11	2.17	0.57
1:F:343:TYR:HE1	1:F:345:ARG:O	1.87	0.57
1:F:385:ARG:HH11	1:F:385:ARG:CB	2.18	0.57
2:H:5:GLU:CG	2:H:9:LYS:HE2	2.35	0.57
2:H:123:GLN:HA	2:H:123:GLN:NE2	2.19	0.57
1:A:290:LEU:HB2	1:A:293:VAL:HG21	1.86	0.56
1:E:310:ILE:HD13	1:E:379:ALA:HB1	1.87	0.56
1:B:154:VAL:HG12	1:B:158:LEU:HD11	1.87	0.56
2:C:114:PRO:HG2	2:C:117:GLU:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:6:LEU:O	2:G:10:LEU:HB2	2.05	0.56
2:G:111:GLU:CD	2:G:111:GLU:H	2.13	0.56
2:H:3:GLN:CD	2:H:6:LEU:CB	2.78	0.56
1:A:335:PHE:CE2	1:A:361:MET:HB2	2.39	0.56
1:B:385:ARG:HH11	1:B:385:ARG:CB	2.18	0.56
2:C:7:ILE:HG23	2:C:25:LEU:CD1	2.36	0.56
2:G:32:GLU:O	2:G:35:ALA:N	2.38	0.56
2:H:42:ARG:HA	2:H:45:MET:CE	2.35	0.56
1:A:278:GLN:CD	1:A:278:GLN:H	2.12	0.56
1:E:295:ARG:HG3	1:E:295:ARG:HH11	1.71	0.56
1:F:267:VAL:HG13	1:F:288:VAL:CG1	2.36	0.56
1:F:320:VAL:CG1	1:F:321:TYR:H	2.17	0.56
1:F:342:PHE:N	1:F:342:PHE:HD1	2.02	0.56
1:A:278:GLN:HG2	1:A:279:GLU:H	1.71	0.56
2:C:33:GLU:CD	2:C:33:GLU:N	2.47	0.56
2:C:34:LYS:N	2:C:34:LYS:CD	2.65	0.56
1:F:16:THR:HG23	1:F:79:HIS:HE1	1.71	0.56
1:F:93:ILE:HD11	1:F:319:SER:OG	2.05	0.56
1:A:385:ARG:HH11	1:A:385:ARG:CG	2.18	0.56
1:B:222:LEU:C	1:B:222:LEU:HD23	2.31	0.56
1:F:95:GLY:HA2	1:F:385:ARG:NE	2.21	0.56
2:G:134:LYS:HB3	2:G:138:ILE:HG21	1.88	0.56
1:F:223:MET:HG3	1:F:242:ILE:HA	1.87	0.56
1:A:313:HIS:HD2	1:A:405:GLU:O	1.89	0.56
2:C:3:GLN:NE2	2:C:30:TRP:CE3	2.74	0.56
2:C:138:ILE:HG22	2:C:139:ALA:N	2.19	0.56
2:D:172:LEU:HD12	2:D:172:LEU:O	2.05	0.56
1:A:171:ILE:N	1:A:171:ILE:CD1	2.69	0.56
1:E:248:LYS:HB3	1:E:279:GLU:HG3	1.88	0.56
2:G:50:LYS:O	2:G:53:ARG:HG2	2.06	0.56
1:B:234:ARG:NH1	2:G:144:GLU:HG2	2.21	0.55
2:H:106:ARG:HD2	2:H:107:TYR:CE1	2.41	0.55
2:C:137:GLN:NE2	2:C:137:GLN:N	2.53	0.55
1:B:342:PHE:HA	1:B:387:ALA:O	2.06	0.55
2:D:118:LEU:HD12	2:D:118:LEU:C	2.31	0.55
1:F:90:LYS:O	1:F:94:THR:HG23	2.06	0.55
2:G:135:PRO:HG2	2:G:138:ILE:HG12	1.89	0.55
2:H:17:GLY:O	2:H:21:VAL:HG23	2.07	0.55
1:B:290:LEU:HD23	1:B:293:VAL:HG21	1.89	0.55
2:D:32:GLU:OE1	2:D:32:GLU:N	2.40	0.55
2:H:5:GLU:O	2:H:9:LYS:HG3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:TYR:CD1	1:A:343:TYR:N	2.75	0.55
1:B:343:TYR:HD2	1:B:389:ARG:NH2	2.05	0.55
1:E:293:VAL:HA	1:E:297:GLU:OE1	2.06	0.55
1:F:267:VAL:HG12	1:F:269:GLY:H	1.71	0.55
2:H:134:LYS:HD2	2:H:134:LYS:N	2.21	0.55
1:B:263:ARG:NH1	1:B:263:ARG:CB	2.70	0.55
1:B:130:TYR:CE1	1:B:164:PRO:HG3	2.42	0.55
2:C:35:ALA:O	2:C:38:LEU:N	2.38	0.55
1:E:301:GLY:HA2	1:E:347:THR:HG22	1.89	0.55
1:E:391:GLY:C	1:E:393:ARG:H	2.14	0.55
1:F:299:GLU:H	1:F:302:GLN:NE2	2.04	0.55
2:H:7:ILE:HG23	2:H:21:VAL:CB	2.37	0.55
2:H:111:GLU:CD	2:H:111:GLU:H	2.14	0.55
1:B:326:GLU:C	1:B:328:GLY:H	2.15	0.55
2:C:100:ILE:HG23	2:C:105:PRO:HD2	1.89	0.55
1:A:146:LEU:O	1:A:150:VAL:HG23	2.06	0.55
1:A:391:GLY:C	1:A:393:ARG:H	2.15	0.55
1:B:289:LEU:O	1:B:290:LEU:HD13	2.06	0.55
1:B:389:ARG:HB2	1:B:393:ARG:O	2.07	0.55
2:C:67:ASN:OD1	2:C:67:ASN:C	2.49	0.55
1:E:267:VAL:HG13	1:E:288:VAL:HG13	1.89	0.55
2:G:10:LEU:HD11	2:G:25:LEU:HD21	1.89	0.54
2:G:50:LYS:NZ	2:G:53:ARG:NH1	2.55	0.54
2:H:57:GLU:O	2:H:77:ASN:HA	2.07	0.54
1:B:299:GLU:H	1:B:302:GLN:NE2	2.04	0.54
2:C:99:HIS:HE1	2:C:159:GLN:OE1	1.90	0.54
1:F:268:THR:HB	1:F:289:LEU:HD12	1.89	0.54
1:F:293:VAL:HG23	1:F:293:VAL:O	2.06	0.54
2:H:130:LEU:HD13	2:H:135:PRO:C	2.31	0.54
1:B:263:ARG:HB3	1:B:263:ARG:NH1	2.20	0.54
1:E:335:PHE:HA	1:E:355:LEU:HD11	1.88	0.54
2:G:4:MET:HE2	2:G:5:GLU:N	2.22	0.54
2:H:8:LYS:HE2	2:H:9:LYS:NZ	2.22	0.54
1:B:263:ARG:HH11	1:B:263:ARG:CB	2.18	0.54
2:C:11:ARG:HB2	2:C:21:VAL:HG21	1.90	0.54
1:F:385:ARG:HH11	1:F:385:ARG:CG	2.20	0.54
2:G:129:ALA:O	2:G:132:GLU:HB2	2.08	0.54
1:B:223:MET:CE	1:B:304:LEU:HD21	2.31	0.54
2:H:3:GLN:HG2	2:H:4:MET:N	2.22	0.54
1:F:335:PHE:CE2	1:F:361:MET:HB2	2.43	0.54
1:A:271:GLU:OE2	1:A:274:ARG:HA	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:GLN:HG3	1:A:348:ASP:OD2	2.07	0.54
1:B:86:ALA:O	1:B:87:ASP:C	2.51	0.54
1:B:171:ILE:N	1:B:171:ILE:CD1	2.70	0.54
2:G:99:HIS:HE1	2:G:159:GLN:OE1	1.91	0.54
1:B:95:GLY:HA2	1:B:385:ARG:CZ	2.37	0.54
1:F:146:LEU:O	1:F:149:LEU:HB3	2.08	0.54
2:C:128:ALA:HA	2:C:131:ASN:HB2	1.89	0.53
1:A:38:GLU:HG3	1:A:200:TRP:CZ2	2.43	0.53
1:B:224:PRO:HD2	1:B:241:ARG:O	2.09	0.53
2:G:121:GLU:O	2:G:124:ILE:HB	2.08	0.53
2:G:192:PHE:CB	2:H:60:ILE:HD12	2.38	0.53
1:A:251:ASP:O	1:A:267:VAL:HG23	2.08	0.53
2:D:57:GLU:O	2:D:77:ASN:HA	2.08	0.53
1:F:385:ARG:HG3	1:F:399:VAL:HG12	1.90	0.53
1:B:146:LEU:O	1:B:149:LEU:HB3	2.08	0.53
1:E:385:ARG:HH11	1:E:385:ARG:HB2	1.72	0.53
1:F:113:MET:HA	1:F:113:MET:HE2	1.89	0.53
2:G:21:VAL:O	2:G:25:LEU:HD12	2.09	0.53
2:G:123:GLN:CA	2:G:126:ILE:HG12	2.38	0.53
1:A:320:VAL:HG12	1:A:321:TYR:H	1.71	0.53
1:B:385:ARG:HH11	1:B:385:ARG:CG	2.22	0.53
2:D:3:GLN:NE2	2:D:3:GLN:H	2.07	0.53
1:E:221:PHE:O	1:E:305:ALA:HB1	2.08	0.53
1:E:347:THR:OG1	1:E:348:ASP:N	2.37	0.53
1:F:171:ILE:N	1:F:171:ILE:CD1	2.71	0.53
2:G:34:LYS:HE3	2:G:34:LYS:H	1.74	0.53
2:H:7:ILE:HG23	2:H:21:VAL:CG1	2.39	0.53
1:B:95:GLY:CA	1:B:385:ARG:NE	2.68	0.53
1:B:385:ARG:HG3	1:B:399:VAL:HG12	1.90	0.53
2:D:3:GLN:OE1	2:D:5:GLU:N	2.42	0.53
1:E:320:VAL:CG1	1:E:321:TYR:N	2.72	0.53
1:B:136:ASN:CG	1:B:137:LYS:H	2.17	0.53
1:B:236:THR:HG21	1:B:295:ARG:N	2.24	0.53
1:E:141:VAL:HG21	1:E:147:LEU:HD21	1.90	0.53
1:E:155:ARG:NH2	1:E:168:VAL:O	2.36	0.53
2:D:10:LEU:HD21	2:D:36:VAL:CG1	2.38	0.53
1:E:115:GLN:HG2	2:G:83:VAL:HG23	1.90	0.53
1:B:236:THR:HG1	1:B:293:VAL:HG23	1.72	0.53
1:B:335:PHE:CE2	1:B:361:MET:HB2	2.44	0.53
2:C:113:ILE:CG2	2:C:114:PRO:HD2	2.39	0.53
1:E:38:GLU:HG3	1:E:200:TRP:CZ2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:313:HIS:HD2	1:E:405:GLU:O	1.92	0.53
2:G:50:LYS:HZ3	2:G:53:ARG:NH1	2.07	0.53
1:A:304:LEU:CD2	1:A:304:LEU:N	2.71	0.52
2:C:17:GLY:O	2:C:20:ASP:N	2.42	0.52
1:F:17:ILE:HG22	1:F:82:CYS:HB2	1.91	0.52
1:F:332:THR:HA	2:G:102:MET:HE2	1.90	0.52
1:A:310:ILE:HD13	1:A:379:ALA:HB1	1.91	0.52
1:B:304:LEU:CD2	1:B:304:LEU:N	2.73	0.52
2:H:125:TYR:HA	2:H:146:ARG:NH1	2.18	0.52
1:B:304:LEU:H	1:B:304:LEU:HD22	1.74	0.52
2:C:57:GLU:O	2:C:77:ASN:HA	2.10	0.52
2:D:67:ASN:C	2:D:67:ASN:OD1	2.52	0.52
1:E:290:LEU:HD22	1:E:290:LEU:H	1.73	0.52
1:A:223:MET:HB3	1:A:304:LEU:HD21	1.90	0.52
1:B:143:ASP:HB2	2:D:22:LYS:NZ	2.24	0.52
2:D:79:GLU:HB2	2:D:182:GLU:OE1	2.08	0.52
1:F:154:VAL:HG12	1:F:158:LEU:HD11	1.91	0.52
1:F:236:THR:HG1	1:F:293:VAL:HG23	1.72	0.52
2:C:121:GLU:HA	2:C:124:ILE:CD1	2.34	0.52
2:C:121:GLU:O	2:C:121:GLU:HG3	2.10	0.52
1:E:385:ARG:CG	1:E:399:VAL:HG12	2.39	0.52
1:F:154:VAL:O	1:F:158:LEU:HD12	2.10	0.52
1:F:301:GLY:HA2	1:F:346:THR:OG1	2.09	0.52
1:B:93:ILE:HD11	1:B:319:SER:OG	2.09	0.52
1:B:350:THR:HB	1:B:375:ILE:HD13	1.92	0.52
1:A:249:VAL:HG12	1:A:250:GLY:N	2.25	0.52
1:E:350:THR:HB	1:E:375:ILE:HD13	1.90	0.52
1:F:146:LEU:HD21	2:H:18:MET:HG3	1.92	0.52
1:B:320:VAL:CG1	1:B:321:TYR:H	2.20	0.52
1:B:343:TYR:CE1	1:B:345:ARG:O	2.63	0.52
2:C:60:ILE:HD12	2:D:192:PHE:HB3	1.90	0.52
2:D:10:LEU:HD11	2:D:39:LEU:CD1	2.40	0.52
2:H:125:TYR:HB3	2:H:143:ALA:CB	2.37	0.52
1:A:236:THR:OG1	1:A:293:VAL:HG23	2.10	0.51
2:G:128:ALA:O	2:G:132:GLU:HG3	2.09	0.51
2:D:119:GLU:C	2:D:121:GLU:N	2.65	0.51
1:F:254:GLU:HG3	1:F:264:ARG:HB3	1.91	0.51
2:H:37:GLN:O	2:H:41:GLU:HB2	2.11	0.51
1:B:75:ARG:HH22	1:B:210:ILE:HG22	1.75	0.51
1:E:115:GLN:HG2	2:G:83:VAL:HG22	1.92	0.51
1:B:86:ALA:HA	1:B:89:ILE:HG22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:GLY:CA	1:B:347:THR:HG22	2.41	0.51
1:E:113:MET:HE2	1:E:113:MET:HA	1.93	0.51
2:G:67:ASN:OD1	2:G:67:ASN:C	2.53	0.51
1:B:95:GLY:HA2	1:B:385:ARG:HE	1.74	0.51
1:B:228:VAL:HG22	1:B:238:ALA:CB	2.40	0.51
1:E:271:GLU:OE2	1:E:274:ARG:HA	2.10	0.51
2:D:114:PRO:HG2	2:D:117:GLU:HB2	1.93	0.51
2:D:148:LYS:O	2:D:152:GLU:HG3	2.10	0.51
1:B:17:ILE:HG22	1:B:82:CYS:HB2	1.91	0.51
1:E:35:THR:HG21	1:E:70:TYR:HB2	1.92	0.51
1:F:231:ILE:HG22	1:F:231:ILE:O	2.10	0.51
1:F:344:PHE:O	1:F:347:THR:HG23	2.11	0.51
2:D:120:LYS:O	2:D:124:ILE:HD11	2.10	0.51
1:E:90:LYS:HE3	1:E:321:TYR:CZ	2.45	0.51
2:G:135:PRO:HB2	2:G:137:GLN:OE1	2.10	0.51
1:F:226:GLU:HB3	1:F:300:ARG:HH21	1.76	0.51
1:B:267:VAL:HG13	1:B:288:VAL:HG13	1.93	0.51
1:B:301:GLY:HA2	1:B:346:THR:OG1	2.11	0.51
1:E:168:VAL:HG13	1:E:169:PRO:HD2	1.93	0.51
1:F:136:ASN:CG	1:F:137:LYS:H	2.19	0.51
1:A:122:LEU:O	1:A:126:VAL:HG13	2.12	0.50
1:B:266:VAL:HB	1:B:291:ARG:NH1	2.25	0.50
2:C:31:ASP:HB3	2:C:34:LYS:HZ1	1.75	0.50
2:C:121:GLU:CA	2:C:124:ILE:HD12	2.34	0.50
2:D:72:VAL:HA	2:D:190:CYS:O	2.12	0.50
1:E:130:TYR:CE2	1:E:209:TYR:HB3	2.46	0.50
1:F:289:LEU:HD23	1:F:289:LEU:H	1.76	0.50
1:A:343:TYR:N	1:A:343:TYR:HD1	2.09	0.50
1:F:85:HIS:ND1	1:F:85:HIS:C	2.69	0.50
2:G:43:GLY:HA2	2:G:46:LYS:HG3	1.92	0.50
2:C:4:MET:O	2:C:6:LEU:N	2.44	0.50
2:C:34:LYS:H	2:C:34:LYS:CD	2.23	0.50
1:F:224:PRO:CA	1:F:303:VAL:HG23	2.38	0.50
1:F:244:ARG:HA	1:F:282:ALA:HB2	1.94	0.50
1:F:271:GLU:HG3	1:F:275:LYS:H	1.77	0.50
1:A:115:GLN:HG2	2:C:83:VAL:CG2	2.41	0.50
1:F:210:ILE:O	1:F:210:ILE:CG1	2.59	0.50
2:H:28:ALA:O	2:H:29:GLY:O	2.30	0.50
1:B:224:PRO:CA	1:B:303:VAL:HG23	2.36	0.50
2:C:113:ILE:HG23	2:C:114:PRO:HD2	1.93	0.50
1:F:75:ARG:NH1	1:F:212:THR:HG23	2.23	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:349:VAL:CG1	1:F:350:THR:N	2.74	0.50
2:H:127:GLN:O	2:H:131:ASN:ND2	2.44	0.50
1:B:95:GLY:HA2	1:B:385:ARG:NE	2.27	0.50
2:C:14:THR:HG22	2:C:40:ARG:HH12	1.75	0.50
2:C:17:GLY:O	2:C:18:MET:C	2.54	0.50
1:F:38:GLU:HG3	1:F:200:TRP:CZ2	2.46	0.50
1:B:155:ARG:NH2	1:B:168:VAL:O	2.40	0.50
1:B:320:VAL:CG1	1:B:321:TYR:N	2.72	0.50
1:B:325:LYS:HD2	1:B:331:HIS:ND1	2.27	0.50
1:B:344:PHE:O	1:B:347:THR:HG23	2.11	0.50
1:E:90:LYS:HE3	1:E:321:TYR:CE1	2.46	0.50
1:E:304:LEU:H	1:E:304:LEU:HD22	1.77	0.50
1:A:17:ILE:HD13	1:A:103:ILE:O	2.12	0.50
2:D:7:ILE:HG23	2:D:21:VAL:HG12	1.93	0.50
1:E:95:GLY:HA2	1:E:385:ARG:NH2	2.20	0.50
1:E:150:VAL:O	1:E:153:GLU:HB2	2.12	0.50
1:E:304:LEU:CD2	1:E:304:LEU:N	2.73	0.50
1:E:343:TYR:OH	1:E:389:ARG:HD2	2.11	0.50
2:G:36:VAL:HG23	2:G:37:GLN:N	2.26	0.50
2:G:68:GLN:HE22	2:H:90:GLN:HE22	1.59	0.50
2:G:136:GLN:O	2:G:137:GLN:C	2.53	0.50
1:B:254:GLU:O	1:B:304:LEU:HA	2.12	0.50
1:E:223:MET:O	1:E:304:LEU:CD2	2.60	0.50
1:F:247:VAL:O	1:F:247:VAL:HG13	2.10	0.50
1:F:298:VAL:C	1:F:299:GLU:HG3	2.36	0.50
1:B:267:VAL:HG13	1:B:288:VAL:CG1	2.42	0.49
2:D:131:ASN:C	2:D:133:GLY:H	2.16	0.49
1:E:17:ILE:HD13	1:E:17:ILE:N	2.27	0.49
1:E:253:VAL:HG22	1:E:254:GLU:H	1.77	0.49
2:G:121:GLU:O	2:G:122:ARG:C	2.54	0.49
1:A:141:VAL:HG21	1:A:147:LEU:HD21	1.94	0.49
1:A:155:ARG:NH2	1:A:168:VAL:O	2.40	0.49
1:A:190:ARG:HD3	1:A:200:TRP:CD1	2.47	0.49
1:B:35:THR:HG21	1:B:70:TYR:HB2	1.94	0.49
2:H:72:VAL:HA	2:H:190:CYS:O	2.11	0.49
2:D:81:ASP:C	2:D:81:ASP:OD1	2.56	0.49
1:E:249:VAL:HG12	1:E:250:GLY:N	2.28	0.49
1:F:185:ASN:HB3	1:F:188:THR:OG1	2.13	0.49
2:G:126:ILE:HD13	2:G:143:ALA:HB2	1.95	0.49
2:H:8:LYS:HE2	2:H:9:LYS:HZ3	1.77	0.49
1:E:151:GLU:O	1:E:155:ARG:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:223:MET:HB3	1:E:304:LEU:HD21	1.94	0.49
2:H:125:TYR:HE2	2:H:147:LEU:N	2.10	0.49
1:B:275:LYS:O	1:B:276:THR:O	2.30	0.49
1:E:17:ILE:HG22	1:E:82:CYS:HB2	1.94	0.49
2:G:3:GLN:O	2:G:30:TRP:CZ3	2.65	0.49
2:H:81:ASP:OD1	2:H:81:ASP:C	2.56	0.49
1:A:17:ILE:HG22	1:A:82:CYS:HB2	1.95	0.49
2:C:7:ILE:O	2:C:10:LEU:N	2.45	0.49
2:H:33:GLU:C	2:H:35:ALA:N	2.66	0.49
2:H:109:SER:HA	2:H:157:LEU:HD23	1.95	0.49
1:E:236:THR:OG1	1:E:293:VAL:HG23	2.13	0.49
1:E:267:VAL:HG13	1:E:288:VAL:CG1	2.42	0.49
1:F:221:PHE:O	1:F:222:LEU:HB2	2.13	0.49
1:F:389:ARG:HB2	1:F:393:ARG:O	2.13	0.49
2:G:10:LEU:CD1	2:G:25:LEU:HD11	2.43	0.49
2:D:28:ALA:O	2:D:29:GLY:O	2.31	0.49
1:B:223:MET:O	1:B:304:LEU:CD2	2.60	0.49
2:C:29:GLY:O	2:C:31:ASP:N	2.41	0.49
1:E:385:ARG:HG3	1:E:385:ARG:NH1	2.28	0.49
1:F:150:VAL:O	1:F:153:GLU:HB2	2.13	0.49
1:B:90:LYS:HE2	1:B:321:TYR:CE1	2.48	0.49
1:B:264:ARG:NH1	1:B:264:ARG:CG	2.71	0.49
1:B:266:VAL:HB	1:B:291:ARG:HH11	1.77	0.49
1:B:349:VAL:CG1	1:B:350:THR:N	2.75	0.49
1:B:361:MET:HE1	2:C:102:MET:CB	2.43	0.49
1:F:146:LEU:O	1:F:150:VAL:HG23	2.12	0.49
1:F:267:VAL:HG13	1:F:288:VAL:HG13	1.94	0.49
1:B:75:ARG:NH1	1:B:212:THR:HG23	2.09	0.48
1:B:146:LEU:HD22	2:D:19:MET:SD	2.53	0.48
1:B:150:VAL:O	1:B:153:GLU:HB2	2.11	0.48
2:C:23:ARG:O	2:C:27:ASP:N	2.38	0.48
2:D:53:ARG:HH11	2:D:53:ARG:HG2	1.78	0.48
1:E:190:ARG:HD3	1:E:200:TRP:CD1	2.48	0.48
1:F:176:LEU:O	1:F:180:GLU:HG3	2.13	0.48
1:F:312:PRO:HA	1:F:378:VAL:O	2.12	0.48
1:A:113:MET:HA	1:A:113:MET:HE2	1.95	0.48
1:A:315:LYS:HA	1:A:372:VAL:O	2.12	0.48
1:B:271:GLU:HG2	1:B:274:ARG:HA	1.94	0.48
2:C:120:LYS:HG2	2:C:124:ILE:HD11	1.94	0.48
2:C:130:LEU:HA	2:C:134:LYS:O	2.14	0.48
1:E:171:ILE:N	1:E:171:ILE:CD1	2.75	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:155:ARG:NH2	1:F:170:VAL:HG23	2.28	0.48
2:H:25:LEU:HD22	2:H:30:TRP:CE3	2.48	0.48
1:A:151:GLU:O	1:A:155:ARG:HG3	2.13	0.48
1:A:248:LYS:HB3	1:A:279:GLU:HG3	1.94	0.48
1:B:272:MET:HB2	1:B:277:LEU:HD12	1.95	0.48
2:C:109:SER:HA	2:C:157:LEU:HD23	1.95	0.48
2:D:92:LEU:HD11	2:D:96:LEU:HD11	1.95	0.48
1:E:141:VAL:HG21	1:E:147:LEU:CD2	2.44	0.48
1:F:253:VAL:CG2	1:F:254:GLU:H	2.21	0.48
1:A:247:VAL:O	1:A:247:VAL:HG13	2.11	0.48
1:B:109:ALA:O	2:D:19:MET:HB2	2.13	0.48
1:B:298:VAL:C	1:B:299:GLU:HG3	2.37	0.48
1:B:343:TYR:CD1	1:B:347:THR:O	2.67	0.48
2:C:34:LYS:O	2:C:38:LEU:HB2	2.13	0.48
2:D:74:VAL:O	2:D:74:VAL:HG13	2.14	0.48
1:F:130:TYR:HE1	1:F:164:PRO:HG2	1.79	0.48
1:F:212:THR:CG2	1:F:213:PRO:HD2	2.43	0.48
2:G:35:ALA:O	2:G:38:LEU:N	2.46	0.48
2:G:81:ASP:OD1	2:G:81:ASP:C	2.56	0.48
2:H:114:PRO:O	2:H:118:LEU:HD12	2.14	0.48
1:A:223:MET:O	1:A:304:LEU:CD2	2.62	0.48
1:A:301:GLY:HA2	1:A:347:THR:HG22	1.96	0.48
1:B:223:MET:HG3	1:B:242:ILE:HA	1.95	0.48
1:F:341:GLN:NE2	1:F:391:GLY:N	2.47	0.48
2:G:125:TYR:CD2	2:G:146:ARG:HB3	2.48	0.48
1:A:222:LEU:HD23	1:A:223:MET:N	2.28	0.48
1:A:335:PHE:HA	1:A:355:LEU:HD11	1.95	0.48
2:C:172:LEU:HD12	2:C:172:LEU:O	2.14	0.48
2:D:27:ASP:CG	2:D:42:ARG:HH22	2.22	0.48
2:D:119:GLU:C	2:D:121:GLU:H	2.21	0.48
2:G:148:LYS:O	2:G:152:GLU:HG3	2.13	0.48
2:H:67:ASN:OD1	2:H:67:ASN:C	2.56	0.48
1:A:304:LEU:H	1:A:304:LEU:HD23	1.79	0.48
2:D:109:SER:HA	2:D:157:LEU:HD23	1.96	0.48
1:A:150:VAL:O	1:A:153:GLU:HB2	2.14	0.48
2:H:92:LEU:HD12	2:H:92:LEU:O	2.14	0.48
1:A:253:VAL:HG22	1:A:254:GLU:H	1.79	0.48
1:B:208:GLU:HB2	1:B:209:TYR:H	1.46	0.48
2:D:4:MET:O	2:D:8:LYS:CB	2.61	0.48
1:E:326:GLU:C	1:E:328:GLY:H	2.22	0.48
2:H:172:LEU:HD12	2:H:172:LEU:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:LEU:HD23	2:D:18:MET:HG3	1.96	0.48
2:H:148:LYS:O	2:H:152:GLU:HG3	2.13	0.48
1:A:350:THR:HB	1:A:375:ILE:CD1	2.44	0.47
2:C:81:ASP:OD1	2:C:81:ASP:C	2.57	0.47
2:C:159:GLN:O	2:C:169:VAL:HG23	2.14	0.47
1:F:35:THR:HG21	1:F:70:TYR:HB2	1.96	0.47
1:F:298:VAL:HA	1:F:302:GLN:NE2	2.12	0.47
2:G:6:LEU:HD23	2:G:25:LEU:CD2	2.43	0.47
1:A:231:ILE:O	1:A:231:ILE:CG2	2.61	0.47
1:A:290:LEU:HD23	1:A:293:VAL:HG21	1.95	0.47
1:A:343:TYR:CE2	1:A:348:ASP:HB2	2.48	0.47
1:E:123:ALA:O	1:E:127:GLY:N	2.47	0.47
1:E:391:GLY:O	1:E:393:ARG:N	2.47	0.47
2:H:125:TYR:CG	2:H:146:ARG:NH1	2.82	0.47
2:C:125:TYR:CE2	2:C:146:ARG:HB3	2.49	0.47
1:E:231:ILE:HG22	1:E:234:ARG:HG3	1.97	0.47
1:A:223:MET:HB3	1:A:304:LEU:CD2	2.45	0.47
1:B:146:LEU:O	1:B:150:VAL:HG23	2.14	0.47
1:B:313:HIS:HB3	1:B:405:GLU:OXT	2.14	0.47
1:E:101:GLY:HA3	1:E:210:ILE:HD13	1.96	0.47
1:F:93:ILE:C	1:F:95:GLY:H	2.22	0.47
1:F:290:LEU:O	1:F:293:VAL:HG22	2.13	0.47
1:A:231:ILE:HD13	1:A:231:ILE:HA	1.71	0.47
2:G:32:GLU:O	2:G:33:GLU:C	2.56	0.47
2:G:100:ILE:HG23	2:G:105:PRO:HD2	1.97	0.47
1:B:38:GLU:HG3	1:B:200:TRP:CZ2	2.48	0.47
1:B:93:ILE:C	1:B:95:GLY:H	2.23	0.47
2:C:137:GLN:HE21	2:C:137:GLN:N	2.06	0.47
1:E:143:ASP:HB3	1:E:146:LEU:HG	1.95	0.47
1:E:315:LYS:HA	1:E:372:VAL:O	2.14	0.47
1:A:231:ILE:O	1:A:232:THR:C	2.57	0.47
1:B:148:ASP:O	1:B:152:MET:HE3	2.14	0.47
1:B:290:LEU:HD22	1:B:290:LEU:H	1.75	0.47
2:C:42:ARG:HA	2:C:45:MET:HE3	1.97	0.47
2:C:72:VAL:HA	2:C:190:CYS:O	2.15	0.47
1:E:253:VAL:HG22	1:E:254:GLU:N	2.30	0.47
1:F:89:ILE:H	1:F:89:ILE:HG12	1.55	0.47
1:F:136:ASN:CG	1:F:137:LYS:N	2.73	0.47
2:G:35:ALA:O	2:G:36:VAL:C	2.58	0.47
2:G:122:ARG:HG2	2:G:126:ILE:HD11	1.96	0.47
2:H:115:ALA:HA	2:H:118:LEU:CD1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:LYS:HE2	1:A:321:TYR:CE1	2.50	0.47
1:A:290:LEU:HD22	1:A:290:LEU:H	1.77	0.47
1:B:154:VAL:O	1:B:155:ARG:C	2.58	0.47
1:B:212:THR:HG22	1:B:213:PRO:HD2	1.95	0.47
1:B:221:PHE:CG	1:B:222:LEU:N	2.83	0.47
1:B:290:LEU:N	1:B:290:LEU:CD2	2.74	0.47
1:B:293:VAL:HG23	1:B:293:VAL:O	2.15	0.47
2:C:92:LEU:HD12	2:C:92:LEU:O	2.14	0.47
2:D:33:GLU:H	2:D:33:GLU:HG2	1.53	0.47
2:D:53:ARG:HG2	2:D:79:GLU:CD	2.40	0.47
1:E:98:GLN:OE1	1:E:98:GLN:HA	2.15	0.47
2:D:116:GLU:H	2:D:116:GLU:HG3	1.51	0.47
2:D:134:LYS:HG3	2:D:142:ILE:CD1	2.44	0.47
1:F:222:LEU:HA	1:F:305:ALA:HB2	1.97	0.47
1:F:225:VAL:HG13	1:F:238:ALA:HB1	1.96	0.47
2:G:147:LEU:HD23	2:G:147:LEU:HA	1.72	0.47
1:A:231:ILE:HG22	1:A:234:ARG:HG3	1.97	0.47
1:A:385:ARG:HH11	1:A:385:ARG:CB	2.27	0.47
2:C:32:GLU:O	2:C:35:ALA:HB3	2.15	0.47
2:C:126:ILE:O	2:C:130:LEU:HG	2.15	0.47
2:G:94:LYS:HA	2:G:94:LYS:HD3	1.60	0.47
2:H:36:VAL:HG23	2:H:37:GLN:N	2.30	0.47
1:E:320:VAL:CG1	1:E:321:TYR:H	2.27	0.46
2:G:50:LYS:NZ	2:G:53:ARG:HH12	2.11	0.46
1:B:368:VAL:CG1	1:B:369:THR:H	2.20	0.46
1:F:216:ASP:HA	1:F:219:LYS:HD2	1.97	0.46
2:H:3:GLN:NE2	2:H:30:TRP:CE3	2.64	0.46
1:A:254:GLU:OE1	1:A:307:PRO:HA	2.15	0.46
1:B:136:ASN:CG	1:B:137:LYS:N	2.72	0.46
2:C:118:LEU:HD12	2:C:118:LEU:C	2.39	0.46
2:C:129:ALA:HB3	2:C:139:ALA:CB	2.45	0.46
2:G:29:GLY:O	2:G:31:ASP:N	2.46	0.46
2:G:33:GLU:O	2:G:37:GLN:HB2	2.15	0.46
1:B:19:HIS:O	1:B:22:HIS:HB2	2.14	0.46
1:E:156:ASP:HA	1:E:159:ASN:HD22	1.80	0.46
1:E:231:ILE:O	1:E:232:THR:C	2.57	0.46
1:E:290:LEU:HD23	1:E:293:VAL:HG21	1.97	0.46
1:F:295:ARG:HG3	1:F:295:ARG:HH11	1.79	0.46
1:A:123:ALA:O	1:A:127:GLY:N	2.49	0.46
1:A:267:VAL:HG13	1:A:288:VAL:HG13	1.97	0.46
1:B:113:MET:HE2	1:B:113:MET:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:ILE:HD12	1:B:263:ARG:NH1	2.31	0.46
1:F:15:GLY:HA3	1:F:99:MET:SD	2.56	0.46
2:G:50:LYS:O	2:G:52:ASP:N	2.49	0.46
2:H:74:VAL:O	2:H:74:VAL:HG13	2.16	0.46
1:A:112:PRO:O	1:A:113:MET:HE2	2.16	0.46
1:B:143:ASP:HB2	2:D:22:LYS:HZ1	1.81	0.46
1:B:270:VAL:HG12	1:B:271:GLU:N	2.30	0.46
2:C:114:PRO:HG2	2:C:117:GLU:CB	2.45	0.46
2:D:135:PRO:HD2	2:D:138:ILE:HD12	1.97	0.46
1:A:298:VAL:C	1:A:299:GLU:HG3	2.41	0.46
2:D:134:LYS:HB2	2:D:138:ILE:CB	2.44	0.46
1:F:353:VAL:HG13	1:F:370:PHE:CD1	2.51	0.46
2:G:72:VAL:HA	2:G:190:CYS:O	2.16	0.46
1:A:168:VAL:HG13	1:A:169:PRO:HD2	1.97	0.46
1:A:198:LYS:O	1:A:201:GLU:HB2	2.15	0.46
1:A:281:ILE:O	1:A:282:ALA:C	2.59	0.46
1:A:295:ARG:HG3	1:A:295:ARG:NH1	2.30	0.46
1:A:304:LEU:H	1:A:304:LEU:HD22	1.79	0.46
1:A:320:VAL:CG1	1:A:321:TYR:N	2.77	0.46
1:B:130:TYR:HE1	1:B:164:PRO:CG	2.29	0.46
1:B:291:ARG:NH1	1:B:291:ARG:HB2	2.30	0.46
1:B:335:PHE:HA	1:B:355:LEU:HD11	1.98	0.46
2:G:58:GLY:O	2:H:194:LEU:CD2	2.64	0.46
2:G:126:ILE:HD13	2:G:126:ILE:H	1.81	0.46
2:H:127:GLN:O	2:H:131:ASN:HB2	2.15	0.46
1:A:143:ASP:HA	1:A:144:PRO:HD3	1.79	0.46
1:A:258:LEU:HD12	1:A:302:GLN:HG3	1.96	0.46
1:B:216:ASP:C	1:B:218:ASP:N	2.74	0.46
1:B:229:PHE:HB2	1:B:230:THR:H	1.57	0.46
1:F:228:VAL:HG21	1:F:298:VAL:CG1	2.35	0.46
1:F:350:THR:HB	1:F:375:ILE:HD13	1.98	0.46
1:A:154:VAL:HG12	1:A:158:LEU:HD11	1.97	0.46
1:A:305:ALA:O	1:A:306:LYS:C	2.59	0.46
1:B:114:PRO:HG2	1:B:115:GLN:HE21	1.81	0.46
1:B:295:ARG:HD3	1:B:295:ARG:C	2.41	0.46
1:B:353:VAL:HG13	1:B:370:PHE:CD1	2.51	0.46
2:C:5:GLU:OE1	2:C:5:GLU:HA	2.16	0.46
2:C:185:VAL:CG1	2:C:186:VAL:N	2.79	0.46
1:F:146:LEU:CD2	2:H:18:MET:HG3	2.46	0.46
1:F:151:GLU:O	1:F:155:ARG:HG3	2.16	0.46
2:G:4:MET:O	2:G:5:GLU:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:123:GLN:NE2	2:H:126:ILE:HG13	2.30	0.46
1:A:154:VAL:O	1:A:158:LEU:HD12	2.17	0.45
2:D:11:ARG:O	2:D:15:GLY:N	2.44	0.45
2:D:86:ASN:OD1	2:D:88:LEU:HB2	2.15	0.45
1:F:210:ILE:O	1:F:211:PRO:C	2.56	0.45
2:G:115:ALA:O	2:G:118:LEU:HB3	2.16	0.45
1:A:385:ARG:HG3	1:A:385:ARG:NH1	2.31	0.45
1:B:133:VAL:HG12	1:B:134:PHE:N	2.30	0.45
2:C:36:VAL:HG23	2:C:37:GLN:N	2.30	0.45
2:C:125:TYR:CD2	2:C:146:ARG:HB3	2.51	0.45
1:E:157:LEU:O	1:E:160:GLN:HB2	2.16	0.45
2:G:123:GLN:HA	2:G:126:ILE:HG13	1.99	0.45
1:A:93:ILE:C	1:A:95:GLY:N	2.74	0.45
1:E:136:ASN:CG	1:E:137:LYS:N	2.74	0.45
1:F:143:ASP:CG	1:F:145:GLU:HB2	2.41	0.45
1:F:326:GLU:C	1:F:328:GLY:N	2.72	0.45
2:G:60:ILE:HD12	2:H:192:PHE:HB3	1.98	0.45
1:A:141:VAL:HG21	1:A:147:LEU:CD2	2.47	0.45
1:B:185:ASN:HB3	1:B:188:THR:OG1	2.16	0.45
1:B:289:LEU:HD23	1:B:289:LEU:H	1.81	0.45
2:C:46:LYS:H	2:C:46:LYS:HG2	1.44	0.45
1:E:93:ILE:C	1:E:95:GLY:N	2.74	0.45
2:G:122:ARG:O	2:G:125:TYR:N	2.50	0.45
1:B:332:THR:HA	2:C:102:MET:HE2	1.99	0.45
1:E:263:ARG:NH2	1:E:297:GLU:HG2	2.32	0.45
1:F:19:HIS:O	1:F:22:HIS:HB2	2.16	0.45
2:G:130:LEU:HD12	2:G:130:LEU:HA	1.80	0.45
2:H:100:ILE:HG23	2:H:105:PRO:HD2	1.97	0.45
2:D:38:LEU:HD12	2:D:38:LEU:HA	1.78	0.45
2:D:133:GLY:O	2:D:134:LYS:C	2.60	0.45
1:E:198:LYS:O	1:E:201:GLU:HB2	2.15	0.45
1:E:385:ARG:CG	1:E:385:ARG:NH1	2.78	0.45
2:H:116:GLU:OE1	2:H:116:GLU:N	2.48	0.45
1:A:17:ILE:HD13	1:A:17:ILE:N	2.30	0.45
1:A:190:ARG:HD3	1:A:200:TRP:CG	2.52	0.45
1:B:176:LEU:O	1:B:180:GLU:HG3	2.17	0.45
2:C:34:LYS:HZ3	2:C:34:LYS:CB	2.30	0.45
2:D:130:LEU:CD1	2:D:135:PRO:HA	2.40	0.45
1:E:190:ARG:HD3	1:E:200:TRP:CG	2.52	0.45
1:E:267:VAL:HG12	1:E:269:GLY:H	1.82	0.45
2:H:7:ILE:HD11	2:H:22:LYS:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:GLU:O	1:A:304:LEU:HA	2.16	0.45
1:A:310:ILE:HG12	1:A:311:THR:N	2.32	0.45
1:B:225:VAL:HG13	1:B:238:ALA:HB1	1.98	0.45
2:C:28:ALA:HB2	2:C:38:LEU:CD2	2.46	0.45
2:C:60:ILE:HD12	2:D:192:PHE:CB	2.47	0.45
1:E:385:ARG:HG3	1:E:385:ARG:HH11	1.80	0.45
1:F:293:VAL:HA	1:F:297:GLU:OE1	2.16	0.45
1:F:347:THR:OG1	1:F:348:ASP:N	2.48	0.45
2:H:6:LEU:O	2:H:25:LEU:HD11	2.17	0.45
2:H:114:PRO:HB2	2:H:116:GLU:CD	2.42	0.45
1:A:222:LEU:HA	1:A:305:ALA:HB2	1.98	0.45
1:A:393:ARG:HE	1:A:393:ARG:HB3	1.60	0.45
1:B:304:LEU:N	1:B:304:LEU:HD22	2.32	0.45
2:G:7:ILE:O	2:G:8:LYS:C	2.59	0.45
2:G:18:MET:HE3	2:G:18:MET:HB2	1.85	0.45
2:H:136:GLN:CD	2:H:136:GLN:C	2.84	0.45
2:H:165:ASP:N	2:H:165:ASP:OD1	2.50	0.45
1:B:109:ALA:HA	2:D:19:MET:CG	2.46	0.45
2:C:120:LYS:HG2	2:C:124:ILE:CD1	2.47	0.45
2:D:164:ASP:C	2:D:166:LYS:H	2.25	0.45
1:A:156:ASP:HA	1:A:159:ASN:HD22	1.82	0.44
2:D:19:MET:HB3	2:D:23:ARG:CZ	2.46	0.44
1:F:299:GLU:H	1:F:302:GLN:HE21	1.65	0.44
2:G:21:VAL:O	2:G:22:LYS:C	2.60	0.44
2:H:94:LYS:HA	2:H:94:LYS:HD3	1.71	0.44
1:A:294:SER:H	1:A:297:GLU:CD	2.25	0.44
1:A:316:PHE:HA	1:A:404:LEU:HG	1.99	0.44
1:B:223:MET:O	1:B:303:VAL:HG22	2.17	0.44
2:G:169:VAL:O	2:G:170:LYS:C	2.58	0.44
1:A:318:ALA:HA	1:A:401:THR:HG23	1.99	0.44
1:B:15:GLY:HA3	1:B:99:MET:SD	2.57	0.44
1:B:86:ALA:C	1:B:89:ILE:HG22	2.43	0.44
2:C:94:LYS:HA	2:C:94:LYS:HD3	1.61	0.44
1:E:112:PRO:O	1:E:113:MET:HE2	2.18	0.44
1:E:228:VAL:HG12	1:E:229:PHE:N	2.33	0.44
1:E:385:ARG:HH11	1:E:385:ARG:CB	2.29	0.44
2:G:135:PRO:O	2:G:138:ILE:HB	2.17	0.44
2:H:36:VAL:O	2:H:39:LEU:HB2	2.18	0.44
2:H:83:VAL:HG21	2:H:182:GLU:CD	2.43	0.44
1:B:199:ILE:O	1:B:202:LEU:HB3	2.17	0.44
1:E:247:VAL:O	1:E:247:VAL:CG1	2.62	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:THR:HG21	1:A:294:SER:C	2.43	0.44
1:A:291:ARG:NH1	1:A:291:ARG:CB	2.80	0.44
1:B:111:GLY:HA2	1:B:150:VAL:HG13	1.99	0.44
2:C:135:PRO:HB2	2:C:137:GLN:HE22	1.82	0.44
1:E:221:PHE:CG	1:E:222:LEU:N	2.86	0.44
1:E:272:MET:HB2	1:E:277:LEU:HD12	2.00	0.44
1:F:130:TYR:HE1	1:F:164:PRO:CG	2.30	0.44
2:H:7:ILE:HG12	2:H:25:LEU:HD13	1.99	0.44
2:H:38:LEU:HD12	2:H:38:LEU:HA	1.90	0.44
1:A:253:VAL:HG22	1:A:254:GLU:N	2.31	0.44
1:B:312:PRO:HA	1:B:378:VAL:O	2.18	0.44
1:B:342:PHE:N	1:B:342:PHE:HD1	2.16	0.44
1:B:361:MET:HE1	2:C:102:MET:HB2	1.99	0.44
2:C:120:LYS:HE2	2:C:124:ILE:HD11	1.99	0.44
2:C:165:ASP:N	2:C:165:ASP:OD1	2.50	0.44
2:G:172:LEU:HD12	2:G:172:LEU:O	2.17	0.44
1:A:265:THR:HG21	1:A:293:VAL:HG13	1.99	0.44
1:B:155:ARG:NH2	1:B:170:VAL:HG23	2.33	0.44
1:B:216:ASP:O	1:B:218:ASP:N	2.51	0.44
1:E:35:THR:O	1:E:36:ALA:C	2.61	0.44
1:E:251:ASP:O	1:E:267:VAL:HG23	2.18	0.44
2:H:11:ARG:HD3	2:H:18:MET:SD	2.58	0.44
2:H:123:GLN:HE22	2:H:126:ILE:HG13	1.82	0.44
2:H:185:VAL:CG1	2:H:186:VAL:N	2.81	0.44
1:B:230:THR:HG22	1:B:235:GLY:O	2.18	0.44
1:B:295:ARG:NH1	1:B:295:ARG:CG	2.79	0.44
2:D:92:LEU:HD12	2:D:92:LEU:O	2.18	0.44
1:E:335:PHE:CZ	1:E:361:MET:HE3	2.53	0.44
1:F:112:PRO:O	1:F:113:MET:HE2	2.18	0.44
2:G:109:SER:HA	2:G:157:LEU:HD23	2.00	0.44
2:H:169:VAL:O	2:H:170:LYS:C	2.60	0.44
2:C:164:ASP:C	2:C:166:LYS:N	2.76	0.43
2:D:165:ASP:OD1	2:D:165:ASP:N	2.51	0.43
1:E:259:ALA:HB1	1:E:260:PRO:HD2	1.99	0.43
1:F:241:ARG:HG2	1:F:242:ILE:O	2.18	0.43
2:G:136:GLN:C	2:G:138:ILE:N	2.75	0.43
2:H:115:ALA:HA	2:H:118:LEU:HD12	1.99	0.43
1:A:188:THR:HG22	1:A:189:ARG:N	2.33	0.43
1:A:393:ARG:O	1:A:395:VAL:HG13	2.17	0.43
1:B:268:THR:HB	1:B:289:LEU:HD12	2.00	0.43
1:B:284:ASP:O	1:B:286:VAL:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:LEU:HD23	1:B:289:LEU:N	2.33	0.43
2:C:4:MET:O	2:C:5:GLU:C	2.61	0.43
2:D:2:SER:HB2	2:D:3:GLN:H	1.54	0.43
2:D:3:GLN:C	2:D:5:GLU:H	2.25	0.43
2:D:123:GLN:C	2:D:125:TYR:N	2.76	0.43
2:D:147:LEU:HD23	2:D:147:LEU:HA	1.81	0.43
1:F:271:GLU:HG2	1:F:274:ARG:HA	2.00	0.43
1:F:291:ARG:HB2	1:F:291:ARG:HH11	1.80	0.43
2:H:86:ASN:OD1	2:H:88:LEU:HB2	2.17	0.43
1:A:12:VAL:HG13	1:A:100:ASP:HB2	1.99	0.43
1:E:254:GLU:O	1:E:304:LEU:HA	2.19	0.43
1:F:200:TRP:O	1:F:201:GLU:C	2.60	0.43
1:F:393:ARG:HE	1:F:393:ARG:HB3	1.66	0.43
2:G:80:THR:HG23	2:G:182:GLU:OE2	2.18	0.43
2:G:90:GLN:HE22	2:H:68:GLN:HE22	1.65	0.43
1:A:115:GLN:HG2	2:C:83:VAL:HG23	2.00	0.43
1:B:264:ARG:HH11	1:B:264:ARG:CG	2.06	0.43
2:C:83:VAL:HG21	2:C:182:GLU:CD	2.44	0.43
2:C:130:LEU:HD21	2:C:136:GLN:HA	1.99	0.43
2:C:164:ASP:C	2:C:166:LYS:H	2.27	0.43
2:C:168:LYS:O	2:C:171:GLU:HB2	2.18	0.43
2:D:62:HIS:HA	2:D:72:VAL:O	2.18	0.43
1:E:294:SER:H	1:E:297:GLU:CD	2.26	0.43
1:F:264:ARG:NH1	1:F:264:ARG:CG	2.76	0.43
1:B:169:PRO:HD3	1:B:209:TYR:CD1	2.54	0.43
1:B:200:TRP:O	1:B:201:GLU:C	2.60	0.43
2:D:17:GLY:O	2:D:20:ASP:N	2.51	0.43
2:D:100:ILE:HG23	2:D:105:PRO:HD2	2.00	0.43
1:F:12:VAL:HG13	1:F:100:ASP:HB2	2.00	0.43
1:F:121:LEU:HG	1:F:161:TYR:CE2	2.53	0.43
1:F:148:ASP:O	1:F:152:MET:HE3	2.18	0.43
1:F:265:THR:HG21	1:F:293:VAL:HG13	2.01	0.43
2:G:126:ILE:HD13	2:G:126:ILE:N	2.33	0.43
1:B:168:VAL:HG13	1:B:169:PRO:HD2	2.01	0.43
1:E:121:LEU:HG	1:E:161:TYR:CE2	2.53	0.43
1:E:223:MET:HB3	1:E:304:LEU:CD2	2.48	0.43
1:E:265:THR:HG21	1:E:293:VAL:HG13	1.99	0.43
1:E:305:ALA:O	1:E:306:LYS:C	2.60	0.43
1:F:182:MET:SD	1:F:188:THR:HB	2.59	0.43
1:A:237:VAL:CG1	1:A:238:ALA:N	2.81	0.43
2:D:18:MET:HE2	2:D:18:MET:HB2	1.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:136:ASN:CG	1:E:137:LYS:H	2.26	0.43
1:E:236:THR:HG1	1:E:293:VAL:HG23	1.83	0.43
1:E:237:VAL:CG1	1:E:238:ALA:N	2.81	0.43
1:E:312:PRO:HA	1:E:378:VAL:O	2.18	0.43
1:F:335:PHE:HA	1:F:355:LEU:HD11	2.00	0.43
2:G:165:ASP:OD1	2:G:165:ASP:N	2.51	0.43
1:B:113:MET:O	1:B:116:THR:HB	2.18	0.43
1:B:146:LEU:CD2	2:D:19:MET:SD	3.07	0.43
1:F:275:LYS:O	1:F:276:THR:O	2.36	0.43
1:A:312:PRO:HA	1:A:378:VAL:O	2.19	0.43
2:C:4:MET:C	2:C:6:LEU:N	2.75	0.43
2:C:7:ILE:O	2:C:9:LYS:N	2.51	0.43
2:D:8:LYS:O	2:D:12:GLU:HB3	2.19	0.43
1:F:133:VAL:HG12	1:F:134:PHE:N	2.33	0.43
1:F:187:LYS:O	1:F:188:THR:C	2.62	0.43
2:G:3:GLN:NE2	2:G:30:TRP:CE3	2.87	0.43
2:G:74:VAL:O	2:G:74:VAL:HG13	2.19	0.43
1:B:88:TYR:CD1	1:B:88:TYR:C	2.97	0.43
1:E:17:ILE:HD13	1:E:103:ILE:O	2.19	0.43
1:F:86:ALA:O	1:F:87:ASP:C	2.62	0.43
2:G:164:ASP:C	2:G:166:LYS:H	2.27	0.43
2:G:168:LYS:O	2:G:169:VAL:C	2.62	0.43
2:C:14:THR:HG21	2:C:40:ARG:HH12	1.82	0.42
2:C:132:GLU:OE2	2:C:134:LYS:HE2	2.18	0.42
2:D:4:MET:HA	2:D:7:ILE:HD12	1.99	0.42
1:F:265:THR:O	1:F:266:VAL:HG23	2.19	0.42
1:F:375:ILE:HG13	1:F:376:LYS:N	2.34	0.42
1:A:39:ASN:HA	1:A:40:PRO:HD2	1.49	0.42
1:A:136:ASN:CG	1:A:137:LYS:N	2.77	0.42
1:A:385:ARG:CG	1:A:385:ARG:NH1	2.79	0.42
1:B:151:GLU:O	1:B:155:ARG:HG3	2.19	0.42
2:C:32:GLU:O	2:C:33:GLU:C	2.62	0.42
2:C:169:VAL:O	2:C:170:LYS:C	2.62	0.42
2:D:135:PRO:HD2	2:D:138:ILE:CD1	2.49	0.42
1:F:89:ILE:O	1:F:90:LYS:C	2.61	0.42
1:B:149:LEU:HB2	2:D:4:MET:HE3	2.01	0.42
1:B:210:ILE:HG22	1:B:210:ILE:O	2.17	0.42
1:B:231:ILE:O	1:B:232:THR:C	2.63	0.42
1:B:326:GLU:C	1:B:328:GLY:N	2.76	0.42
2:D:45:MET:HE3	2:D:45:MET:HB2	1.91	0.42
1:F:222:LEU:HD23	1:F:222:LEU:C	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:368:VAL:CG1	1:F:369:THR:H	2.18	0.42
2:H:84:ALA:HA	2:H:89:PHE:CD2	2.54	0.42
1:A:214:VAL:HG12	1:A:218:ASP:HB2	2.01	0.42
1:A:271:GLU:HG2	1:A:274:ARG:HA	2.02	0.42
1:A:311:THR:OG1	1:A:313:HIS:CE1	2.72	0.42
1:B:85:HIS:H	2:D:81:ASP:CG	2.28	0.42
2:C:121:GLU:O	2:C:124:ILE:HB	2.19	0.42
2:D:7:ILE:HG23	2:D:21:VAL:CG1	2.49	0.42
1:F:85:HIS:O	1:F:89:ILE:HG12	2.19	0.42
2:G:126:ILE:HA	2:G:139:ALA:HB1	2.01	0.42
2:G:132:GLU:OE1	2:G:134:LYS:NZ	2.44	0.42
2:G:146:ARG:HH11	2:G:146:ARG:CG	2.17	0.42
2:H:80:THR:HG23	2:H:182:GLU:CD	2.44	0.42
1:A:267:VAL:HG12	1:A:269:GLY:H	1.84	0.42
1:B:112:PRO:O	1:B:113:MET:HE2	2.19	0.42
1:B:149:LEU:O	1:B:150:VAL:C	2.62	0.42
1:B:361:MET:CE	2:C:102:MET:HB2	2.49	0.42
2:C:92:LEU:HD11	2:C:96:LEU:HD11	2.01	0.42
1:E:100:ASP:O	1:E:129:PRO:HG2	2.20	0.42
1:E:237:VAL:HG12	1:E:238:ALA:N	2.32	0.42
1:E:393:ARG:HE	1:E:393:ARG:HB3	1.60	0.42
2:H:109:SER:HB2	2:H:111:GLU:OE2	2.19	0.42
1:A:193:ASN:OD1	1:A:196:VAL:HG23	2.19	0.42
1:B:130:TYR:CE1	1:B:164:PRO:CG	3.01	0.42
1:E:154:VAL:O	1:E:158:LEU:HD12	2.20	0.42
2:G:31:ASP:OD1	2:G:34:LYS:NZ	2.48	0.42
2:H:135:PRO:HB2	2:H:136:GLN:H	1.73	0.42
1:B:12:VAL:CG1	1:B:13:ASN:N	2.83	0.42
1:B:188:THR:HG22	1:B:189:ARG:N	2.35	0.42
1:B:271:GLU:HG3	1:B:275:LYS:H	1.84	0.42
2:C:74:VAL:O	2:C:74:VAL:HG13	2.19	0.42
2:D:3:GLN:C	2:D:5:GLU:N	2.78	0.42
2:D:28:ALA:C	2:D:29:GLY:O	2.62	0.42
1:F:138:VAL:O	1:F:141:VAL:HG13	2.20	0.42
2:G:53:ARG:HG2	2:G:53:ARG:H	1.57	0.42
2:G:194:LEU:CD2	2:H:58:GLY:O	2.67	0.42
1:A:237:VAL:CG2	1:A:289:LEU:HB3	2.44	0.42
1:B:115:GLN:CG	2:D:83:VAL:HG22	2.47	0.42
2:C:185:VAL:HG12	2:C:186:VAL:N	2.35	0.42
1:F:16:THR:CG2	1:F:79:HIS:HE1	2.31	0.42
1:F:117:ARG:HG3	1:F:161:TYR:OH	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:109:SER:HB2	2:G:111:GLU:OE2	2.20	0.42
2:H:79:GLU:HB2	2:H:182:GLU:OE1	2.20	0.42
2:H:164:ASP:C	2:H:166:LYS:H	2.28	0.42
1:A:237:VAL:HG12	1:A:238:ALA:N	2.34	0.42
1:B:12:VAL:HG22	1:B:213:PRO:CD	2.50	0.42
1:B:223:MET:O	1:B:304:LEU:HD23	2.19	0.42
1:B:268:THR:HG1	1:B:291:ARG:HG3	1.81	0.42
1:E:304:LEU:H	1:E:304:LEU:HD23	1.82	0.42
1:F:147:LEU:N	1:F:147:LEU:HD23	2.35	0.42
2:G:83:VAL:HG21	2:G:182:GLU:CD	2.45	0.42
2:G:92:LEU:HD11	2:G:96:LEU:HD11	2.02	0.42
2:H:80:THR:HG23	2:H:182:GLU:OE2	2.20	0.42
1:B:85:HIS:O	1:B:89:ILE:HB	2.20	0.42
2:D:78:CYS:SG	2:D:83:VAL:HG12	2.60	0.42
2:D:148:LYS:O	2:D:152:GLU:CG	2.68	0.42
1:E:143:ASP:HA	1:E:144:PRO:HD3	1.78	0.42
1:F:81:ASP:O	1:F:83:PRO:HD3	2.20	0.42
2:G:6:LEU:HD23	2:G:25:LEU:HD22	2.02	0.42
1:A:199:ILE:O	1:A:202:LEU:HB3	2.20	0.41
1:A:335:PHE:CZ	1:A:361:MET:HE3	2.55	0.41
1:B:168:VAL:CG2	1:B:209:TYR:OH	2.68	0.41
1:B:275:LYS:O	1:B:276:THR:C	2.63	0.41
1:B:281:ILE:O	1:B:282:ALA:C	2.63	0.41
2:C:120:LYS:HB3	2:C:120:LYS:NZ	2.35	0.41
2:D:110:ALA:O	2:D:113:ILE:HG13	2.20	0.41
1:E:69:GLU:HG2	1:E:76:HIS:NE2	2.35	0.41
1:E:268:THR:O	1:E:268:THR:HG22	2.20	0.41
1:E:295:ARG:HG3	1:E:295:ARG:NH1	2.34	0.41
1:E:304:LEU:HD23	1:E:304:LEU:O	2.20	0.41
2:G:123:GLN:C	2:G:126:ILE:HG12	2.44	0.41
1:A:272:MET:HE2	1:A:273:HIS:CE1	2.55	0.41
1:B:216:ASP:C	1:B:218:ASP:H	2.28	0.41
1:B:343:TYR:HE1	1:B:345:ARG:O	2.03	0.41
2:C:11:ARG:NE	2:C:16:ALA:O	2.53	0.41
1:E:12:VAL:HG13	1:E:100:ASP:HB2	2.02	0.41
1:E:130:TYR:CD2	1:E:209:TYR:HB3	2.55	0.41
1:E:188:THR:HG22	1:E:189:ARG:N	2.35	0.41
1:A:80:VAL:HG12	1:A:81:ASP:H	1.85	0.41
1:A:275:LYS:O	1:A:276:THR:C	2.63	0.41
1:A:349:VAL:CG1	1:A:350:THR:N	2.81	0.41
1:B:12:VAL:HG13	1:B:100:ASP:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:180:ILE:HG22	2:C:182:GLU:N	2.36	0.41
2:D:185:VAL:CG1	2:D:186:VAL:N	2.83	0.41
1:E:81:ASP:O	1:E:83:PRO:HD3	2.19	0.41
1:E:281:ILE:O	1:E:282:ALA:C	2.63	0.41
1:F:289:LEU:HD23	1:F:289:LEU:N	2.35	0.41
2:G:19:MET:HB3	2:G:23:ARG:CZ	2.50	0.41
1:A:98:GLN:OE1	1:A:98:GLN:HA	2.15	0.41
1:B:86:ALA:HA	1:B:89:ILE:CG2	2.50	0.41
2:C:3:GLN:HA	2:C:6:LEU:HD12	2.03	0.41
2:C:31:ASP:C	2:C:34:LYS:HZ2	2.27	0.41
2:D:84:ALA:HA	2:D:89:PHE:CD2	2.55	0.41
1:E:141:VAL:CG2	1:E:147:LEU:HD21	2.49	0.41
1:F:154:VAL:O	1:F:155:ARG:C	2.62	0.41
1:A:311:THR:OG1	1:A:313:HIS:HE1	2.04	0.41
2:C:58:GLY:O	2:D:194:LEU:CD2	2.68	0.41
2:D:114:PRO:HG2	2:D:117:GLU:CB	2.50	0.41
1:E:200:TRP:O	1:E:201:GLU:C	2.63	0.41
1:F:111:GLY:HA2	1:F:150:VAL:HG13	2.01	0.41
2:G:159:GLN:O	2:G:169:VAL:HG23	2.20	0.41
1:A:221:PHE:HA	1:A:245:GLY:HA3	2.02	0.41
1:B:299:GLU:H	1:B:302:GLN:HE21	1.68	0.41
2:C:7:ILE:H	2:C:7:ILE:HG12	1.35	0.41
2:C:11:ARG:O	2:C:15:GLY:N	2.53	0.41
2:C:109:SER:HB2	2:C:111:GLU:OE2	2.20	0.41
2:D:3:GLN:H	2:D:3:GLN:CD	2.29	0.41
2:D:164:ASP:C	2:D:166:LYS:N	2.78	0.41
2:G:31:ASP:CG	2:G:34:LYS:HZ2	2.29	0.41
2:G:42:ARG:HA	2:G:45:MET:CE	2.49	0.41
1:A:263:ARG:HG2	1:A:263:ARG:HH11	1.86	0.41
1:B:222:LEU:HA	1:B:305:ALA:HB2	2.02	0.41
2:C:14:THR:O	2:C:15:GLY:C	2.63	0.41
2:C:147:LEU:HD23	2:C:147:LEU:HA	1.72	0.41
2:D:53:ARG:HG2	2:D:53:ARG:NH1	2.36	0.41
2:D:120:LYS:O	2:D:124:ILE:CD1	2.69	0.41
1:E:80:VAL:HG12	1:E:81:ASP:H	1.86	0.41
1:A:228:VAL:HG12	1:A:229:PHE:N	2.36	0.41
1:A:268:THR:HG22	1:A:268:THR:O	2.21	0.41
1:A:272:MET:HB2	1:A:277:LEU:HD12	2.01	0.41
1:B:223:MET:O	1:B:303:VAL:CG2	2.68	0.41
1:E:275:LYS:O	1:E:276:THR:C	2.63	0.41
1:F:291:ARG:CZ	1:F:291:ARG:CB	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:164:ASP:C	2:G:166:LYS:N	2.76	0.41
2:H:148:LYS:O	2:H:152:GLU:CG	2.69	0.41
1:A:115:GLN:HG2	2:C:83:VAL:HG22	2.02	0.41
1:A:130:TYR:HB3	1:A:209:TYR:HE2	1.82	0.41
1:B:187:LYS:O	1:B:188:THR:C	2.64	0.41
1:B:208:GLU:O	1:B:209:TYR:C	2.63	0.41
1:B:304:LEU:H	1:B:304:LEU:HD23	1.85	0.41
2:D:94:LYS:HA	2:D:94:LYS:HD3	1.72	0.41
1:E:298:VAL:C	1:E:299:GLU:HG3	2.46	0.41
1:E:310:ILE:HG12	1:E:311:THR:N	2.36	0.41
1:E:391:GLY:C	1:E:393:ARG:N	2.79	0.41
1:F:270:VAL:O	1:F:271:GLU:HB2	2.21	0.41
1:F:299:GLU:O	1:F:300:ARG:C	2.64	0.41
2:G:92:LEU:O	2:G:92:LEU:HD12	2.21	0.41
2:G:122:ARG:C	2:G:126:ILE:HD11	2.46	0.41
2:H:4:MET:HE2	2:H:4:MET:HB3	1.93	0.41
2:H:92:LEU:HD11	2:H:96:LEU:HD11	2.03	0.41
1:A:11:HIS:CD2	1:A:76:HIS:CD2	3.08	0.41
1:A:110:ASP:O	2:C:11:ARG:NH2	2.41	0.41
1:A:304:LEU:HD23	1:A:304:LEU:O	2.21	0.41
1:B:89:ILE:HD12	1:B:89:ILE:HA	1.77	0.41
1:B:149:LEU:HD22	2:D:4:MET:HB2	2.03	0.41
1:F:297:GLU:O	1:F:298:VAL:HG23	2.21	0.41
1:F:361:MET:HE1	2:G:102:MET:HB2	2.02	0.41
1:B:81:ASP:O	1:B:83:PRO:HD3	2.22	0.40
1:B:94:THR:C	1:B:96:ALA:H	2.29	0.40
1:B:95:GLY:H	1:B:385:ARG:HE	1.59	0.40
2:G:192:PHE:HB3	2:H:60:ILE:CD1	2.49	0.40
2:H:194:LEU:HD12	2:H:194:LEU:HA	1.82	0.40
1:A:18:GLY:HA2	1:A:119:HIS:CD2	2.56	0.40
2:C:21:VAL:O	2:C:22:LYS:C	2.64	0.40
2:D:10:LEU:HD13	2:D:10:LEU:C	2.46	0.40
1:E:130:TYR:HE1	1:E:164:PRO:HG2	1.87	0.40
1:E:316:PHE:HA	1:E:404:LEU:HG	2.03	0.40
1:A:200:TRP:O	1:A:201:GLU:C	2.64	0.40
1:B:117:ARG:HG3	1:B:161:TYR:OH	2.21	0.40
1:B:216:ASP:HA	1:B:219:LYS:CD	2.50	0.40
2:D:19:MET:HE3	2:D:23:ARG:NH1	2.37	0.40
1:E:221:PHE:HA	1:E:245:GLY:HA3	2.03	0.40
1:E:222:LEU:HA	1:E:305:ALA:HB2	2.02	0.40
1:F:254:GLU:HG2	1:F:262:THR:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:ALA:HB1	1:A:260:PRO:HD2	2.02	0.40
2:C:192:PHE:CB	2:D:60:ILE:HD12	2.50	0.40
2:D:35:ALA:O	2:D:38:LEU:N	2.53	0.40
2:D:169:VAL:O	2:D:170:LYS:C	2.64	0.40
1:E:304:LEU:HD22	1:E:304:LEU:N	2.36	0.40
1:F:115:GLN:CG	2:H:83:VAL:HG22	2.48	0.40
1:F:143:ASP:HA	1:F:144:PRO:HD3	1.81	0.40
2:H:164:ASP:C	2:H:166:LYS:N	2.80	0.40
1:B:221:PHE:HE1	1:B:242:ILE:HG23	1.86	0.40
2:D:28:ALA:HB2	2:D:38:LEU:HD22	2.02	0.40
2:D:70:VAL:HA	2:D:192:PHE:O	2.22	0.40
2:D:134:LYS:CB	2:D:138:ILE:HD12	2.48	0.40
1:E:291:ARG:NH1	1:E:291:ARG:CB	2.83	0.40
2:G:180:ILE:HG22	2:G:182:GLU:N	2.37	0.40
2:G:185:VAL:CG1	2:G:186:VAL:N	2.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	369/405 (91%)	327 (89%)	34 (9%)	8 (2%)	5	26
1	B	369/405 (91%)	308 (84%)	46 (12%)	15 (4%)	2	13
1	E	368/405 (91%)	319 (87%)	39 (11%)	10 (3%)	4	22
1	F	368/405 (91%)	308 (84%)	46 (12%)	14 (4%)	2	15
2	C	193/196 (98%)	164 (85%)	20 (10%)	9 (5%)	2	11
2	D	193/196 (98%)	161 (83%)	25 (13%)	7 (4%)	2	16
2	G	193/196 (98%)	162 (84%)	20 (10%)	11 (6%)	1	8
2	H	192/196 (98%)	165 (86%)	20 (10%)	7 (4%)	2	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2245/2404 (93%)	1914 (85%)	250 (11%)	81 (4%)	2 16

All (81) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	276	THR
1	B	67	HIS
1	B	232	THR
1	B	276	THR
2	C	29	GLY
2	D	132	GLU
1	E	276	THR
1	F	232	THR
1	F	276	THR
2	G	29	GLY
2	G	32	GLU
2	G	136	GLN
2	G	137	GLN
2	H	29	GLY
2	H	134	LYS
1	A	95	GLY
1	B	96	ALA
2	C	5	GLU
2	C	8	LYS
2	C	27	ASP
2	C	30	TRP
2	C	32	GLU
2	C	33	GLU
2	D	27	ASP
2	D	29	GLY
1	E	95	GLY
1	E	247	VAL
1	F	309	SER
2	G	51	ALA
2	H	32	GLU
2	H	135	PRO
1	A	96	ALA
1	A	247	VAL
1	A	345	ARG
1	B	208	GLU
1	B	340	PRO
1	B	345	ARG

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Mol	Chain	Res	Type
2	C	35	ALA
2	D	135	PRO
1	E	345	ARG
1	F	96	ALA
1	F	98	GLN
1	F	220	PRO
1	F	300	ARG
1	F	345	ARG
2	G	30	TRP
2	G	33	GLU
2	G	127	GLN
2	H	51	ALA
1	A	232	THR
1	B	330	ARG
2	C	4	MET
1	E	37	ALA
1	E	96	ALA
1	E	232	THR
1	F	222	LEU
1	F	330	ARG
1	F	340	PRO
2	G	27	ASP
2	H	131	ASN
1	B	215	ARG
2	D	51	ALA
2	D	116	GLU
2	D	164	ASP
1	B	95	GLY
1	B	98	GLN
1	E	98	GLN
1	E	340	PRO
1	F	95	GLY
2	G	8	LYS
2	H	27	ASP
1	B	217	VAL
1	E	392	GLY
1	F	247	VAL
1	A	392	GLY
1	B	213	PRO
1	F	10	PRO
2	G	138	ILE
1	A	340	PRO

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Mol	Chain	Res	Type
1	B	10	PRO
1	B	247	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	306/339 (90%)	259 (85%)	47 (15%)	2	13
1	B	306/339 (90%)	241 (79%)	65 (21%)	1	6
1	E	308/339 (91%)	263 (85%)	45 (15%)	3	15
1	F	302/339 (89%)	242 (80%)	60 (20%)	1	7
2	C	157/162 (97%)	114 (73%)	43 (27%)	0	2
2	D	150/162 (93%)	114 (76%)	36 (24%)	1	4
2	G	157/162 (97%)	122 (78%)	35 (22%)	1	5
2	H	152/162 (94%)	114 (75%)	38 (25%)	0	3
All	All	1838/2004 (92%)	1469 (80%)	369 (20%)	1	7

All (369) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ILE
1	A	20	VAL
1	A	32	THR
1	A	69	GLU
1	A	79	HIS
1	A	89	ILE
1	A	98	GLN
1	A	106	VAL
1	A	115	GLN
1	A	121	LEU
1	A	124	ARG
1	A	126	VAL
1	A	138	VAL

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Mol	Chain	Res	Type
1	A	141	VAL
1	A	142	ASP
1	A	155	ARG
1	A	158	LEU
1	A	166	ASP
1	A	171	ILE
1	A	176	LEU
1	A	214	VAL
1	A	217	VAL
1	A	231	ILE
1	A	239	THR
1	A	248	LYS
1	A	252	GLU
1	A	254	GLU
1	A	263	ARG
1	A	264	ARG
1	A	277	LEU
1	A	278	GLN
1	A	289	LEU
1	A	290	LEU
1	A	299	GLU
1	A	304	LEU
1	A	332	THR
1	A	341	GLN
1	A	343	TYR
1	A	347	THR
1	A	348	ASP
1	A	352	VAL
1	A	361	MET
1	A	374	LEU
1	A	382	GLU
1	A	385	ARG
1	A	393	ARG
1	A	399	VAL
1	B	17	ILE
1	B	20	VAL
1	B	32	THR
1	B	65	THR
1	B	69	GLU
1	B	74	LYS
1	B	89	ILE
1	B	98	GLN

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Mol	Chain	Res	Type
1	B	106	VAL
1	B	115	GLN
1	B	121	LEU
1	B	126	VAL
1	B	130	TYR
1	B	137	LYS
1	B	138	VAL
1	B	141	VAL
1	B	142	ASP
1	B	146	LEU
1	B	152	MET
1	B	155	ARG
1	B	166	ASP
1	B	171	ILE
1	B	172	ARG
1	B	176	LEU
1	B	208	GLU
1	B	210	ILE
1	B	212	THR
1	B	215	ARG
1	B	217	VAL
1	B	229	PHE
1	B	230	THR
1	B	232	THR
1	B	239	THR
1	B	248	LYS
1	B	252	GLU
1	B	254	GLU
1	B	256	VAL
1	B	263	ARG
1	B	264	ARG
1	B	278	GLN
1	B	286	VAL
1	B	289	LEU
1	B	290	LEU
1	B	295	ARG
1	B	299	GLU
1	B	302	GLN
1	B	303	VAL
1	B	304	LEU
1	B	309	SER
1	B	310	ILE

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Mol	Chain	Res	Type
1	B	311	THR
1	B	314	THR
1	B	332	THR
1	B	342	PHE
1	B	347	THR
1	B	348	ASP
1	B	352	VAL
1	B	361	MET
1	B	368	VAL
1	B	374	LEU
1	B	376	LYS
1	B	382	GLU
1	B	385	ARG
1	B	399	VAL
1	B	405	GLU
2	C	3	GLN
2	C	4	MET
2	C	5	GLU
2	C	6	LEU
2	C	7	ILE
2	C	8	LYS
2	C	10	LEU
2	C	11	ARG
2	C	18	MET
2	C	23	ARG
2	C	27	ASP
2	C	33	GLU
2	C	34	LYS
2	C	37	GLN
2	C	40	ARG
2	C	45	MET
2	C	46	LYS
2	C	50	LYS
2	C	54	GLU
2	C	83	VAL
2	C	94	LYS
2	C	103	MET
2	C	111	GLU
2	C	116	GLU
2	C	117	GLU
2	C	119	GLU
2	C	120	LYS

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Mol	Chain	Res	Type
2	C	122	ARG
2	C	123	GLN
2	C	127	GLN
2	C	134	LYS
2	C	137	GLN
2	C	138	ILE
2	C	140	GLU
2	C	141	LYS
2	C	147	LEU
2	C	154	VAL
2	C	157	LEU
2	C	162	VAL
2	C	167	VAL
2	C	175	GLN
2	C	179	LYS
2	C	180	ILE
2	D	2	SER
2	D	3	GLN
2	D	4	MET
2	D	5	GLU
2	D	14	THR
2	D	23	ARG
2	D	27	ASP
2	D	32	GLU
2	D	33	GLU
2	D	45	MET
2	D	46	LYS
2	D	50	LYS
2	D	56	ARG
2	D	83	VAL
2	D	94	LYS
2	D	103	MET
2	D	111	GLU
2	D	116	GLU
2	D	117	GLU
2	D	118	LEU
2	D	122	ARG
2	D	123	GLN
2	D	125	TYR
2	D	126	ILE
2	D	130	LEU
2	D	132	GLU

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Mol	Chain	Res	Type
2	D	134	LYS
2	D	138	ILE
2	D	141	LYS
2	D	154	VAL
2	D	157	LEU
2	D	162	VAL
2	D	167	VAL
2	D	175	GLN
2	D	179	LYS
2	D	180	ILE
1	E	17	ILE
1	E	20	VAL
1	E	32	THR
1	E	69	GLU
1	E	79	HIS
1	E	98	GLN
1	E	106	VAL
1	E	115	GLN
1	E	121	LEU
1	E	126	VAL
1	E	138	VAL
1	E	141	VAL
1	E	142	ASP
1	E	155	ARG
1	E	158	LEU
1	E	166	ASP
1	E	167	GLU
1	E	176	LEU
1	E	215	ARG
1	E	217	VAL
1	E	231	ILE
1	E	239	THR
1	E	248	LYS
1	E	252	GLU
1	E	254	GLU
1	E	263	ARG
1	E	264	ARG
1	E	277	LEU
1	E	278	GLN
1	E	289	LEU
1	E	290	LEU
1	E	293	VAL

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Mol	Chain	Res	Type
1	E	299	GLU
1	E	303	VAL
1	E	304	LEU
1	E	332	THR
1	E	347	THR
1	E	352	VAL
1	E	361	MET
1	E	374	LEU
1	E	382	GLU
1	E	385	ARG
1	E	393	ARG
1	E	399	VAL
1	E	405	GLU
1	F	17	ILE
1	F	20	VAL
1	F	24	LYS
1	F	32	THR
1	F	69	GLU
1	F	74	LYS
1	F	79	HIS
1	F	89	ILE
1	F	106	VAL
1	F	115	GLN
1	F	121	LEU
1	F	126	VAL
1	F	138	VAL
1	F	141	VAL
1	F	142	ASP
1	F	146	LEU
1	F	152	MET
1	F	155	ARG
1	F	166	ASP
1	F	168	VAL
1	F	171	ILE
1	F	172	ARG
1	F	176	LEU
1	F	210	ILE
1	F	212	THR
1	F	214	VAL
1	F	215	ARG
1	F	217	VAL
1	F	223	MET

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Mol	Chain	Res	Type
1	F	229	PHE
1	F	230	THR
1	F	232	THR
1	F	239	THR
1	F	248	LYS
1	F	252	GLU
1	F	254	GLU
1	F	256	VAL
1	F	264	ARG
1	F	278	GLN
1	F	286	VAL
1	F	289	LEU
1	F	299	GLU
1	F	302	GLN
1	F	303	VAL
1	F	306	LYS
1	F	310	ILE
1	F	311	THR
1	F	332	THR
1	F	342	PHE
1	F	347	THR
1	F	348	ASP
1	F	352	VAL
1	F	361	MET
1	F	368	VAL
1	F	374	LEU
1	F	376	LYS
1	F	382	GLU
1	F	385	ARG
1	F	393	ARG
1	F	399	VAL
2	G	3	GLN
2	G	6	LEU
2	G	8	LYS
2	G	10	LEU
2	G	14	THR
2	G	18	MET
2	G	23	ARG
2	G	31	ASP
2	G	34	LYS
2	G	37	GLN
2	G	46	LYS

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Mol	Chain	Res	Type
2	G	50	LYS
2	G	56	ARG
2	G	83	VAL
2	G	94	LYS
2	G	103	MET
2	G	111	GLU
2	G	120	LYS
2	G	126	ILE
2	G	130	LEU
2	G	134	LYS
2	G	137	GLN
2	G	138	ILE
2	G	140	GLU
2	G	141	LYS
2	G	144	GLU
2	G	146	ARG
2	G	147	LEU
2	G	154	VAL
2	G	157	LEU
2	G	162	VAL
2	G	167	VAL
2	G	175	GLN
2	G	179	LYS
2	G	180	ILE
2	H	3	GLN
2	H	5	GLU
2	H	8	LYS
2	H	9	LYS
2	H	10	LEU
2	H	23	ARG
2	H	25	LEU
2	H	33	GLU
2	H	37	GLN
2	H	41	GLU
2	H	46	LYS
2	H	50	LYS
2	H	54	GLU
2	H	56	ARG
2	H	83	VAL
2	H	94	LYS
2	H	103	MET
2	H	106	ARG

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Mol	Chain	Res	Type
2	H	111	GLU
2	H	117	GLU
2	H	118	LEU
2	H	119	GLU
2	H	122	ARG
2	H	123	GLN
2	H	126	ILE
2	H	127	GLN
2	H	131	ASN
2	H	132	GLU
2	H	134	LYS
2	H	141	LYS
2	H	142	ILE
2	H	146	ARG
2	H	157	LEU
2	H	162	VAL
2	H	167	VAL
2	H	175	GLN
2	H	179	LYS
2	H	180	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	HIS
1	A	13	ASN
1	A	76	HIS
1	A	79	HIS
1	A	91	ASN
1	A	115	GLN
1	A	119	HIS
1	A	125	GLN
1	A	159	ASN
1	A	183	HIS
1	A	302	GLN
1	A	313	HIS
1	A	367	ASN
1	B	11	HIS
1	B	13	ASN
1	B	115	GLN
1	B	119	HIS
1	B	159	ASN

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Mol	Chain	Res	Type
1	B	183	HIS
1	B	302	GLN
2	C	3	GLN
2	C	90	GLN
2	C	99	HIS
2	C	137	GLN
2	C	183	ASN
2	D	90	GLN
2	D	99	HIS
2	D	123	GLN
2	D	131	ASN
2	D	183	ASN
1	E	11	HIS
1	E	13	ASN
1	E	79	HIS
1	E	91	ASN
1	E	115	GLN
1	E	119	HIS
1	E	125	GLN
1	E	183	HIS
1	E	302	GLN
1	E	313	HIS
1	E	341	GLN
1	E	367	ASN
1	F	11	HIS
1	F	13	ASN
1	F	19	HIS
1	F	79	HIS
1	F	115	GLN
1	F	119	HIS
1	F	159	ASN
1	F	183	HIS
1	F	302	GLN
1	F	341	GLN
1	F	367	ASN
2	G	3	GLN
2	G	90	GLN
2	G	99	HIS
2	G	127	GLN
2	G	183	ASN
2	H	37	GLN
2	H	90	GLN

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Mol	Chain	Res	Type
2	H	99	HIS
2	H	123	GLN
2	H	136	GLN
2	H	183	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	373/405 (92%)	-0.06	9 (2%) 59 36	25, 50, 91, 109	0
1	B	373/405 (92%)	0.75	21 (5%) 30 15	45, 94, 109, 110	0
1	E	372/405 (91%)	-0.18	4 (1%) 78 57	20, 46, 84, 110	0
1	F	372/405 (91%)	1.09	68 (18%) 3 2	34, 96, 110, 110	0
2	C	195/196 (99%)	-0.05	0 100 100	23, 60, 90, 100	0
2	D	195/196 (99%)	0.32	6 (3%) 51 30	31, 75, 109, 110	0
2	G	195/196 (99%)	-0.16	1 (0%) 87 72	18, 49, 91, 104	0
2	H	194/196 (98%)	0.39	10 (5%) 33 17	23, 76, 109, 110	0
All	All	2269/2404 (94%)	0.30	119 (5%) 33 17	18, 67, 109, 110	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	253	VAL	7.1
1	B	253	VAL	5.8
1	B	78	SER	4.6
1	F	256	VAL	4.5
1	F	262	THR	4.2
1	F	229	PHE	4.0
1	A	40	PRO	3.9
1	E	66	ALA	3.9
1	F	280	GLY	3.9
1	F	272	MET	3.8
1	E	40	PRO	3.7
1	F	276	THR	3.6
1	F	287	GLY	3.5
1	F	277	LEU	3.4
1	F	380	LEU	3.3
1	F	270	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
2	H	38	LEU	3.2
1	F	254	GLU	3.2
1	F	66	ALA	3.2
1	F	346	THR	3.2
2	H	28	ALA	3.2
2	H	45	MET	3.1
1	F	304	LEU	3.1
2	D	2	SER	3.1
1	A	97	ALA	3.1
1	B	103	ILE	3.1
1	F	101	GLY	3.0
1	F	252	GLU	3.0
1	F	222	LEU	2.9
1	F	238	ALA	2.9
2	H	178	ALA	2.9
1	F	288	VAL	2.9
1	B	30	ALA	2.9
1	F	269	GLY	2.9
1	B	231	ILE	2.9
1	F	273	HIS	2.9
1	A	66	ALA	2.9
2	H	35	ALA	2.9
1	F	301	GLY	2.9
1	F	149	LEU	2.9
1	F	312	PRO	2.8
1	F	274	ARG	2.8
1	F	267	VAL	2.8
1	F	316	PHE	2.8
1	F	305	ALA	2.8
1	F	67	HIS	2.8
1	F	379	ALA	2.8
2	H	37	GLN	2.8
1	F	237	VAL	2.7
2	H	31	ASP	2.7
1	A	68	VAL	2.7
1	F	257	GLY	2.7
1	F	351	GLY	2.6
1	F	68	VAL	2.6
1	F	331	HIS	2.6
1	F	224	PRO	2.6
1	F	374	LEU	2.6
1	F	268	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	350	THR	2.6
2	D	4	MET	2.5
1	F	223	MET	2.5
1	F	303	VAL	2.5
1	B	70	TYR	2.4
2	H	4	MET	2.4
1	F	263	ARG	2.4
1	F	275	LYS	2.4
1	F	249	VAL	2.4
1	B	66	ALA	2.4
1	B	40	PRO	2.4
2	D	30	TRP	2.4
1	B	276	THR	2.3
1	F	313	HIS	2.3
2	H	27	ASP	2.3
1	B	232	THR	2.3
1	F	265	THR	2.3
1	B	229	PHE	2.3
1	B	213	PRO	2.3
1	F	255	ILE	2.3
1	F	97	ALA	2.3
1	E	67	HIS	2.3
1	B	81	ASP	2.3
1	F	264	ARG	2.3
1	F	308	GLY	2.3
1	F	212	THR	2.3
1	F	243	GLU	2.3
1	F	319	SER	2.3
1	F	344	PHE	2.3
2	D	123	GLN	2.3
1	B	194	GLU	2.2
1	F	381	GLU	2.2
1	F	142	ASP	2.2
1	B	379	ALA	2.2
2	H	15	GLY	2.2
1	A	74	LYS	2.2
1	F	221	PHE	2.2
1	F	236	THR	2.2
2	D	45	MET	2.2
1	F	143	ASP	2.2
1	A	98	GLN	2.1
1	F	108	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	235	GLY	2.1
1	A	227	ASP	2.1
1	F	247	VAL	2.1
1	A	235	GLY	2.1
1	B	97	ALA	2.1
1	F	110	ASP	2.1
1	F	152	MET	2.1
1	F	310	ILE	2.1
2	D	16	ALA	2.1
1	B	278	GLN	2.1
1	B	377	PRO	2.1
2	G	116	GLU	2.1
1	B	352	VAL	2.0
1	F	309	SER	2.0
1	E	79	HIS	2.0
1	B	23	GLY	2.0
1	B	287	GLY	2.0
1	A	391	GLY	2.0
1	F	283	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.